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ANALYSIS OF THE DISPERSION MODEL EQUATION
IN ITS SEMI-DISCRETE FORM

BY



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A THESIS

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled, "Analysis of the Dispersion Model Equation in its Semi-Discrete Form" submitted by Hardev Singh Koonar, B.Sc. Chemical Engg., in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

ABSTRACT

The partial differential equation describing the transient case of conductive-convective heat transfer or convective mass transfer in homogeneous or non-homogeneous media can be approximated by a set of first order ordinary differential equations if the space derivatives are replaced by approximate finite difference expressions. The concentrations (or temperatures) at a number of discrete points are treated as dependent variables, whereas time is an independent variable in this set of ordinary differential equations. If the medium properties are dependent upon position only, but not on concentration (or temperature), then a set of linear differential equations is obtained. A general method of solution to the problem has been developed, by using certain linear algebra operations, in terms of the matrix describing the spatial distribution of the properties in the media and the vectors describing the initial and boundary conditions.

The solution has been tested for various one dimensional and two dimensional models in homogeneous as well as non-homogeneous media. It has been found that the two dimensional homogeneous and non-homogeneous models closely approximate the one-dimensional homogeneous model for a two-fold variation in Peclet no. and a value of d_p/d_T (particle diameter/tube diameter) upto 0.075.

The solution to the one-dimensional homogeneous model has also been obtained using the higher order correct monotone type finite difference formulations. In the absence of an analytical solution to the various models, the results of different grid spacings have been compared to get an overall idea about the accuracy. In many problems, where the magnitude of the convective term is large, backward difference formulations have been used. The accuracy of the backward difference scheme and the central difference scheme for the convective term has been tested using an analytical solution corresponding to some other set of boundary conditions. It has been found that for a value of the dispersion group greater than one half of the grid spacing, the central difference formulation for the convective term is better but below or equal to this value, the backward difference formulation must be used.

Three types of different input signals have been tried as example problems. The data of frequency response has been generated using four different values of ω (frequency); a relatively simple model has been developed. The best fit parameters of the model have been calculated using quasilinearization.

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I. INTRODUCTION

Dispersion models are used mainly to represent the flow of fluids in empty tubes and packed beds. The physical representation of these models lies in between the plug flow and the back mix flow and a diffusional process. Various types of models can be used to characterize the flow patterns within the process vessels. The models which incorporate mixing in actual flow and a diffusional process are called DISPERSION MODELS. The various dispersion models are represented in the excellent treatise of Bischoff and Levenspiel (5, 20). The various model parameters and the simplifying assumptions are also described there.

The concept of axial dispersion and radial dispersion is analogous to that of diffusion. The methods for finding out these dispersion coefficients are also summarized in (20). In the classical treatment of Bischoff and Levenspiel (20), the various dispersion models are described, from the most general to the most simple. They developed analytical solutions for simple models corresponding to some particular set of boundary conditions. Analytical solutions for non-homogeneous media are not derived in their work. However, the media properties i.e. axial dispersion coefficients and the radial dispersion coefficient

are not uniform but are some functions of its space coordinates and concentration.

The dispersion models are used to predict the behaviour of actual process vessels. The choice of a satisfactory model depends upon the fact how closely the model represents the actual flow. If a flow model closely reflects a real situation, its predicted response curves will closely match the tracer response curves of the real vessel. In the case of empty tubes, the mixing is caused by molecular diffusion and eddy diffusion superimposed on the velocity profile effect. In packed beds the mixing is caused both by splitting of the fluid streams as they go around the particles and by the variations in the velocity across the bed. The dispersion models lend themselves to relatively simple mathematical formulations, analogous to the classical methods of heat conduction and diffusion. In general the dispersion models work well for both empty tubes and packed beds but have different parameters.

The development of computers in the recent past has made practicable another alternative approach of solving this problem, namely the techniques of numerical integration. The various finite difference formulations have been put forward by various investigators (22, 23) for the spatial discretization of the space variables. These give rise to a set of difference differential equations which in turn gives

rise to a matrix differential equation. The integration of this matrix differential equation can be performed either analytically or numerically. The integral term in the analytical solution to the semi-discrete form of the dispersion model equation has been evaluated for various input signals, using analytical procedure of integration. A significant progress has been achieved in this field of numerical analysis during the past few years.

The advantage of the semi-analytical technique over the analytical one is; that a change in the initial condition can be incorporated easily in the semi-analytical technique as compared to the analytical one. One of the main advantages of the numerical methods is that the non-homogenities in the media can be handled with great ease. On the other hand these methods lack generality. If there is a change of initial or boundary conditions, the entire solution has to be repeated. The semi-analytical technique has been used in this work to get the solution of the various dispersion models. The theory of matrices and linear algebra is used to a great extent for a particular mathematical model of the physical system. The coefficient matrix is unsymmetric and the technique used in (23) has been employed to convert this matrix to the real symmetric form. This matrix (symmetric) has distinct eigenvalues and a set of orthogonal eigenvectors associated with it. Using the finite difference scheme

suggested by Price (22), the coefficient matrix obtained was of the monotone type*. This matrix has also distinct, positive eigenvalues but not a set of orthogonal eigenvectors. Depending upon the magnitude of the convective term, the various types of finite difference approximations are used. The concept of radial symmetry has been employed in the case of two dimensional models.

In the remaining chapters of this investigation the above-mentioned concepts are further developed. Chapter II deals with the general theory and a mathematical background of the solution. Chapter III deals with the solution of some simple and complex dispersion models corresponding to certain sets of boundary conditions. Chapter IV deals with the solution of one dimensional model using higher order correct monotone type formulations (22) and the significance of the convective term (24), and some conclusions have been derived from this work in Chapter V.

* A real $(n \times n)$ matrix $A^* = (a^*_{ij})$ is monotone if and only if it possesses a non-negative inverse, i.e. $A^{*-1} \geq 0$.

II. GENERAL THEORY

The general problem of solving the dispersion model partial differential equation is discussed in this chapter. A semi-analytical solution has been developed using some operational methods of linear algebra and matrix algebra.

The general dispersion model which describes the process is derived in the comprehensive treatise of Bischoff and Levenspiel (5). The simplifying assumption is that of constant density. The general dispersion model equation written in the standard vector notation is:

$$\frac{\partial c}{\partial t} + \underline{u} \cdot \nabla c = \nabla \cdot (D \cdot \nabla c) + S + r_c \quad (\text{II.1})$$

where c = The concentration at any point in the reactor.

\underline{u}^* = The velocity vector at a particular point with respect to an arbitrary chosen position.

D = The dispersion coefficient, generally a function of fluid properties and the flow characteristics.

t = Time.

S = The source term.

r_c = The chemical reaction term.

* A bar under a letter is used to denote vector or matrix. Capital letters used for matrices and lower case for vectors.

The general dispersion model equation in cylindrical coordinates is given by:

$$\frac{\partial c}{\partial t} + \underline{u}(r) \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} (D_L(r) \frac{\partial c}{\partial x}) + \frac{1}{r} \frac{\partial}{\partial r} (r D_R(r) \frac{\partial c}{\partial r}) + S + r_c \quad (\text{II.2})$$

The above equation is restricted to the bulk flow in the axial direction and radial symmetry.

where c = The concentration at any point in the reactor.

$\underline{u}(r)$ = Velocity vector at a particular point with respect to an arbitrary position.

$D_L(r)$ = The axial dispersion coefficient.

$D_R(r)$ = The radial dispersion coefficient.

r = The radial position variable.

x = The axial position variable.

Equation (II.1) is a parabolic partial differential equation in four independent variables (time t and three space variables) and one dependent variable c . If D is independent of c , this equation becomes linear, since it contains only the first power of the concentration and its derivatives. Since it contains second partial space derivatives of concentration, it is of the second order. Similar argument holds for equation (II.2) except it has two independent space variables.

The general problem is to determine the concentration profile in the reactor at any time given:

- (i) The concentration distribution at an earlier instant (generally at $t = 0$); this is termed an initial condition.
- (ii) The influence of surroundings on the boundaries of the reactor, these are termed as boundary conditions.

The various types of methods used for the solution can be broadly classified in three main categories.

- (1) Analytical Methods.
- (2) Semi-Analytical Methods.
- (3) Numerical Methods.

The analytical solutions corresponding to one dimensional case are available in (4, 17) for some limited sets of boundary conditions. Carslaw and Jeager (7) deal with some analytical solutions of the conduction type equation. The analytical solutions in the transformed space are available in (3, 13) corresponding to some boundary conditions. The analysis of the experimental study done by Shemilt and Krishnaswamy (26) corresponding to both sets of boundary conditions (same as used in this work) shows that there is no appreciable difference in the

two sets of boundary conditions in the transformed space. The present work is a step to get the solutions of these cases in the time domain.

The numerical methods for solving such type of partial differential equations have been extensively developed since the high speed computers came into existence. The various numerical methods can be mainly classified in two broad categories, namely the explicit and implicit methods. Varga (29) generalized the various methods and developed some general criteria for the stability of these methods. These methods are summarized and stable procedures have been developed for these techniques in (1, 2).

Using numerical methods a general solution can not be obtained. If a slight change is made in the initial and boundary conditions, the whole solution has to be repeated. In the case of numerical methods the integration procedure is stepwise, which is a time-consuming procedure. The solution has to be evaluated at all the previous time intervals to get the solution at the time required.

The semi-analytical solution used in this work for the solution of the dispersion model combines many advantages of the numerical and analytical methods while reducing some of the disadvantages of these methods.

The semi-analytical method uses concept of finite difference approximations, commonly used in numerical analysis along with some matrix theory and operational methods of linear algebra. These methods are not altogether new but the application of these methods to the chemical engineering problem has been limited. Varga (28) suggested the solution of the diffusion type equation using this method. The important work of Wei and Prater (32) also makes use of this method.

By using semi-discrete central finite difference approximations for discretizing the space variables, the equations (II.1) and (II.2) can be brought to the following standard matrix notation form.

$$\underline{G} \frac{d\underline{c}(\theta)}{d\theta} = -\underline{A}^* \underline{c}(\theta) + \underline{s}'(\theta) \quad (\text{II.3})$$

where \underline{G} = A diagonal matrix of constants.

$\underline{c}(\theta)$ = Concentration vector.

\underline{A}^* = Coefficient matrix of constants.

$\underline{s}'(\theta)$ = Boundary condition vector.

θ = Reduced time.

However, the matrix \underline{A}^* is now no longer symmetric and it may or may not be diagonally dominant. To illustrate, consider one dimensional case where the coefficients are constants. i.e.

$$* \quad \frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} \quad (\text{II.4})$$

(a) Using central difference semi-discrete formulations:

$$\frac{\partial^2 c}{\partial z^2} = \frac{c_{i+1}(\theta) - 2c_i(\theta) + c_{i-1}(\theta)}{h^2} \quad (\text{II.5})$$

$$\frac{\partial c}{\partial z} = \frac{c_{i+1}(\theta) - c_{i-1}(\theta)}{2h} \quad (\text{II.6})$$

The typical boundary conditions are:

$$\begin{aligned} \text{I.c} \quad c &= 0 \quad \text{at} \quad \theta = 0 \quad 0 \leq z \leq 1 \\ \text{B.c} \quad c &= 1 \quad \text{at} \quad z = 0 \quad \theta > 0 \end{aligned} \quad (\text{II.7})$$

$$\frac{\partial c}{\partial z} = 0 \text{ at } z = 1$$

The coefficient matrix \underline{A}^* is of the following type:

$$\underline{A}^* = \begin{bmatrix} 2\alpha & -(\alpha + \frac{h}{2}) & \dots\dots\dots \\ -(\alpha + \frac{h}{2}) & 2\alpha & -(\alpha - \frac{h}{2}) & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ & & -(\alpha + \frac{h}{2}) & 2\alpha & -(\alpha - \frac{h}{2}) \\ & & & -(\alpha + \frac{h}{2}) & (\alpha + \frac{h}{2}) \end{bmatrix} \quad (\text{II.8})$$

* For derivation and conversion to the dimensionless form (II.4) refer to Chapter III.

Price, Varga and Warren (23) have shown that the eigenvalues of \underline{A}^* are only real if $\frac{h}{2} < \alpha$ (where h = grid spacing and α = axial dispersion group). If $\frac{h}{2} > \alpha$ then some of the eigenvalues of \underline{A}^* will be complex, leading to oscillating solutions. Such type of solutions would be unacceptable on physical grounds and any matrix differential equation so formulated would represent an inherently incorrect approximation to the original partial differential equation.

If h is chosen such that $\frac{h}{2} < \alpha$, then matrix \underline{A}^* has the following properties:

- (i) All the off diagonal elements are negative.
 - (ii) All the eigenvalues of \underline{A}^* are real and positive and the eigenvectors are also real.
 - (iii) It is a positive definite matrix.
- (b) Using the higher order correct monotone type finite difference formulations as suggested by Price (22).

The computational molecules and the finite difference formulations are given in Chapter IV. The coefficient matrix \underline{A}^* obtained for this case is of the following type:

$$\underline{A}^* = \begin{bmatrix} 24\alpha & -12(\alpha - \frac{h}{2}) & & & \\ -16(\alpha + \frac{h}{2}) & 30\alpha & -16(\alpha - \frac{h}{2}) & (\alpha - h) & \\ (\alpha + h) & -16(\alpha + \frac{h}{2}) & 30\alpha & -16(\alpha - \frac{h}{2}) & (\alpha - h) \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ & & (\alpha + h) & -16(\alpha + \frac{h}{2}) & 30\alpha & -(15\alpha - 7h) \\ & & & (\alpha + h) & (-15\alpha + 9h) & (14\alpha + 8h) \end{bmatrix} \quad (\text{II.9})$$

Although the matrix \underline{A}^* in this case is not diagonally dominant, yet it has the following properties:

- (i) It is monotone (22)*.
- (ii) All the eigenvalues are real, positive and distinct.
- (iii) The eigenvectors are also real.

If the central difference formula is to be used for the convective term, then the requirement is simply that all the off-diagonal elements must be either zero or positive. In many problems of this type where the convective term is large, the above requirement means a mesh spacing so fine that an inordinately large number of grid points must be used. For such cases, Price et al (24) suggests the following second order correct backward difference

* A real (n x n) matrix $\underline{A}^* = (a^*_{i,j})$ is monotone if and only if it possesses a non-negative inverse, i.e. $A^{*-1} \geq 0$.

approximation for the convective term.

$$\frac{\partial c}{\partial z} = \frac{0.5 c_{i-2} - 2 c_{i-1} + 1.5 c_i}{h} \quad (\text{II.10})$$

Equation (II.10) may be used for all grid points except for those next to the boundary where one has to be satisfied with first order correct expressions.

(c) Using monotone type approximations (22) combined with the backward difference scheme for the convective term (24):

The set of boundary conditions used in deriving the coefficient matrix for (b) and (c) is same as given by (II.7). The coefficient matrix \underline{A}^* obtained for this case is of the following type:

$$\underline{A}^* = \begin{bmatrix} (24\alpha+12h) & -12\alpha & & & \\ -(16\alpha+24h) & (30\alpha+18h) & -16\alpha & \alpha & \\ (\alpha+6h) & -(16\alpha+24h) & (30\alpha+18h) & -16\alpha & \alpha \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots & \dots\dots\dots \\ & & (\alpha+6h) & (16\alpha+24h) & (30\alpha+18h) & -15\alpha \\ & & & (\alpha+6h) & -(15\alpha+24h) & (14\alpha+18h) \end{bmatrix} \quad (\text{II.11})$$

The properties of this matrix are same as that of the matrix in (b).

Premultiplying equation (II.3) by \underline{D}^{-1} where \underline{D} = a diagonal matrix with diagonal entries having alternate signs i.e.

$$d_i = (-1)^i |d_i|$$

$$\therefore \underline{D}^{-1} \underline{G} \frac{d\underline{c}(\theta)}{d\theta} = -\underline{D}^{-1} \underline{A}^* \underline{c}(\theta) + \underline{D}^{-1} \underline{s}'(\theta) \quad (\text{II.12})$$

Define a new variable $\underline{v}(\theta)$ as given by (II.13):

$$\underline{c}(\theta) = \underline{D} \underline{v}(\theta) \quad (\text{II.13})$$

Substituting the value of $\underline{c}(\theta)$ in (II.12) gives:

$$\underline{D}^{-1} \underline{G} \underline{D} \frac{d\underline{v}(\theta)}{d\theta} = -\underline{D}^{-1} \underline{A}^* \underline{D} \underline{v}(\theta) + \underline{D}^{-1} \underline{s}'(\theta) \quad (\text{II.14})$$

$$\underline{G}^* \frac{d\underline{v}(\theta)}{d\theta} = -\underline{A} \underline{v}(\theta) + \underline{s}(\theta) \quad (\text{II.15})$$

$$\text{where } \underline{G}^* = \underline{D}^{-1} \underline{G} \underline{D} \quad (\text{II.16})$$

$$\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D} \quad (\text{II.17})$$

$$\underline{s}(\theta) = \underline{D}^{-1} \underline{s}'(\theta) \quad (\text{II.18})$$

The matrices \underline{G}^* and \underline{A} as given by (II.16) and (II.17) are said to undergo a similarity transformation. The matrix \underline{G}^* is again a diagonal matrix and the matrix \underline{A} is now a real, symmetric matrix derived from the original coefficient matrix using similarity transformation as given by (II.17).

From the nature of the problem it is quite evident that \underline{G}^* is a positive real diagonal matrix and hence its inverse \underline{G}^{*-1} exists. Define two new matrices $\underline{G}^{*1/2}$ and $\underline{G}^{*-1/2}$ to denote the diagonal matrices whose elements are the square roots of the elements of \underline{G}^* and \underline{G}^{*-1} respectively.

The derivation of equation (II.3) from (II.1) or (II.2) is discussed at a later stage taking into consideration a number of models.

A new variable $\underline{u}(\theta)$ is defined by the equation (II.19)

$$\underline{u}(\theta) = \underline{G}^{*1/2} \underline{v}(\theta) \quad (\text{II.19})$$

which gives

$$*\underline{v}(\theta) = \underline{G}^{*-1/2} \underline{u}(\theta) \quad (\text{II.20})$$

Substitution of equation (II.20) in (II.15) and premultiplication by $\underline{G}^{*-1/2}$ gives:

$$\frac{d\underline{u}(\theta)}{d\theta} = -\underline{B} \underline{u}(\theta) + \underline{s}^*(\theta) \quad (\text{II.21})$$

where

$$\underline{B} = \underline{G}^{*-1/2} \underline{A} \underline{G}^{*-1/2} \quad (\text{II.22})$$

$$\underline{s}^*(\theta) = \underline{G}^{*-1/2} \underline{s}(\theta) \quad (\text{II.23})$$

* In many cases it will be seen that $\underline{G}^* = \underline{I}$, the identity matrix which makes $\underline{u}(\theta) = \underline{v}(\theta)$.

On the basis of equation (II.21) two types of problems can be posed.

- (1) Given the coefficient matrix \underline{B} , an initial condition vector $\underline{c}(0)$ and the boundary condition vector $\underline{s}'(\theta)$, evaluate the concentration profiles at various elapsed times. This type of problem is known as the "FORWARD PROBLEM".
- (2) Given the concentration profiles $\underline{c}(\theta)$ for various elapsed times and the boundary condition vector $\underline{s}'(\theta)$, calculate the coefficient matrix \underline{B} . The problem of this type is known as the "INVERSE PROBLEM".

In the present work, only the first case has been investigated in detail for a variety of problems. The method used here is based on the semi-discrete form (II.21) of the dispersion model equation. The method used is general and the mathematics of the problem is rigorous. Any type of spatial variation of properties can be approximated; the accuracy being dependent on the mesh size. Any time dependent linear boundary conditions can be handled.

The theory of the forward problem can be divided into the following sections:

- (1) Derivation of the equation in the semi-discrete form.
- (2) Solution of the semi-discrete dispersion model equation.
- (3) Derivation of matrix D used for the conversion of the original coefficient matrix to the real symmetric form.

1. As discussed in chapter III, the partial differential equation representing one dimensional homogeneous problem is:

$$D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} \quad (\text{II.24})$$

The above equation can be converted into the following dimensionless form:

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} \quad (\text{II.25})^*$$

The equation (II.25) is discretized using the central difference semi-discrete finite difference approximations as given by (II.5) and (II.6). The typical initial and boundary conditions are:

$$\left. \begin{array}{l} \text{I.c} \quad c = 0 \text{ at } \theta = 0 \\ \text{B.c} \quad c = a_1 \text{ at } z = 0 \\ \quad \quad \frac{\partial c}{\partial z} = a_2 \text{ at } z = 1 \end{array} \right] \quad (\text{II.26})$$

* For details of the derivation and the meaning of the various symbols refer to Chapter III.

The various boundary condition sets used are also given in Chapter III. The distance $0 \leq z \leq 1$ of the reactor is divided into a finite number of distance increments (n) of equal width h, with an increment of width $\frac{h}{2}$ next to the boundary, where the boundary condition is specified. The grid spacing used is shown in figure II-a. The concentrations at each of these grid points is specified by $c_1, c_2, c_3, \dots, c_n^*$.

Substitution of the set of finite difference expressions into the partial differential equation (II.25) gives a general equation, representing a set of difference differential equations, of the following type:

$$\frac{dc_i}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_{i-1} - 2\alpha c_i + \left(\alpha - \frac{h}{2}\right) c_{i+1} \right] \quad (\text{II.27})$$

Using equation (II.27), a set of ordinary differential equations can now be written to describe the transient process:

$$\frac{dc_1}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) a_1 - 2\alpha c_1 + \left(\alpha - \frac{h}{2}\right) c_2 \right] \quad (\text{II.27.1})$$

$$\frac{dc_2}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_1 - 2\alpha c_2 + \left(\alpha - \frac{h}{2}\right) c_3 \right] \quad (\text{II.27.2})$$

\vdots \vdots \vdots \vdots

* $\bar{C}(\theta)$ is referred to as $w(\theta)$ in chapter III and a foot note is also made there regarding their same meaning.

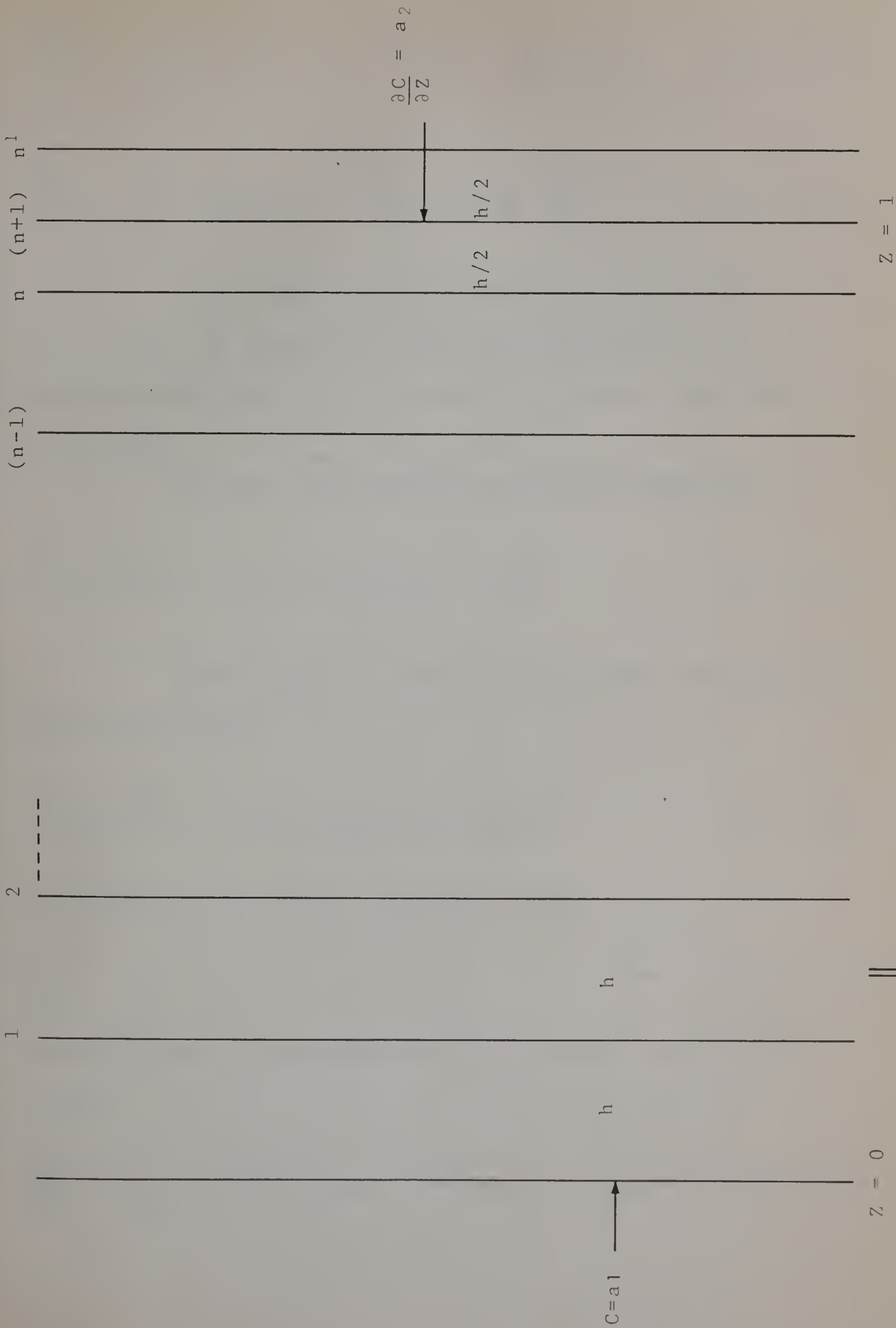


FIGURE II-a
TYPICAL GRID SPACING ONE DIMENSIONAL HOMOGENEOUS CASE

$$\frac{dc_{n-1}}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_{n-2} - 2\alpha c_{n-1} + \left(\alpha - \frac{h}{2}\right) c_n \right] \quad (\text{II.27}(n-1))$$

$$\frac{dc_n}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_{n-1} - 2\alpha c_n + \left(\alpha - \frac{h}{2}\right) c'_n \right] \quad (\text{II.27}.n')$$

Using the boundary condition as specified by (II.26), an expression for concentration at the hypothetical point, c'_n in terms of c_n can be obtained as follows:

At $(n+1)$ the boundary condition specifies:

$$\frac{c_n - c_{n+1}}{h/2} = a_2 \text{ or } c_{n+1} = c_n - a_2 \frac{h}{2} \quad (\text{II.27}(n+1))$$

Also from the conservation of mass, the following expression holds:

$$\frac{c_{n+1} - c'_n}{h/2} = a_2 \text{ or } c_{n+1} = c'_n + a_2 \frac{h}{2} \quad (\text{II.27}(n+2))$$

Combining the last two equations gives:

$$c'_n = c_n - a_2 h \quad (\text{II.27}.(n+3))$$

Substitution of the equation (II.27.(n+3)) in (II.27.n') gives:

$$\frac{dc_n}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_{n-1} - \left(\alpha + \frac{h}{2}\right) c_n \right] - \frac{a_2}{h} \left(\alpha - \frac{h}{2}\right) \quad (\text{II.27}.n)$$

The equations (II.27.1) through (II.27.n) can be represented in the form of a single matrix differential equation as follows:

$$\frac{d}{d\theta} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = -1/h^2 \begin{bmatrix} 2\alpha & -(\alpha - \frac{h}{2}) & & \\ -(\alpha + \frac{h}{2}) & 2\alpha & -(\alpha - \frac{h}{2}) & \\ & \dots\dots\dots & & \\ & & (\alpha + \frac{h}{2}) & 2\alpha & (\alpha - \frac{h}{2}) \\ & & & -(\alpha + \frac{h}{2}) & (\alpha + \frac{h}{2}) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} + \frac{1}{h^2} \begin{bmatrix} (\alpha + \frac{h}{2}) a_1 \\ \vdots \\ -a_2 h (\alpha - \frac{h}{2}) \end{bmatrix} \quad (\text{II.28})$$

Equation (II.28) may also be written as:

$$\frac{d\underline{c}(\theta)}{d\theta} = - \underline{A}^* \underline{c}(\theta) + \underline{s}'(\theta) \quad (\text{II.29})$$

The above equation is same as (II.3) and it has been transformed into equation (II.21) as discussed earlier and the equation is:

$$\frac{d\underline{u}(\theta)}{d\theta} = -\underline{B} \underline{u}(\theta) + \underline{s}^*(\theta) \quad (\text{II.30})$$

2. The solution of the forward problem is a general solution of the equation (II.30) with the initial condition $\underline{u}(0) = \underline{u}_0$.

Since the matrix \underline{B} is a real symmetric and positive definite matrix, it is quite evident that*,

- (i) \underline{B} has n real, positive eigenvalues (n is the order of the matrix) and,
- (ii) \underline{B} has n real and mutually orthogonal eigenvectors q_j ($j = 1, \text{ to } n$) and these satisfy the following relation:

$$q_j q_i = 0 \quad \text{if } i \neq j \quad (\text{II.31})$$

If the eigenvectors are chosen in such a way that they are of unit length, then they are orthonormal which makes:

$$\underline{Q}^{-1} = \underline{Q}^T \quad (\text{II.32})$$

where \underline{Q} = eigenvector matrix of \underline{B} , whose columns are normalized eigenvectors q_j , superscript T refers to the transpose.

This particular fashion for the choice of eigenvectors makes \underline{Q} an orthogonal matrix.

* For proofs refer to Appendix A.

Define a new variable \underline{m} given by the equation (II.33).

$$\underline{m}(\theta) = \underline{Q}^T \underline{u}(\theta) \quad \text{and} \quad \underline{u}(\theta) = \underline{Q} \underline{m}(\theta) \quad (\text{II.33})$$

Replacement of $\underline{u}(\theta)$ by $\underline{m}(\theta)$ in equation (II.30) gives:

$$\underline{Q} \frac{d\underline{m}(\theta)}{d\theta} = - \underline{B} \underline{Q} \underline{m}(\theta) + \underline{S}^* (\theta) \quad (\text{II.34})$$

Premultiplication by \underline{Q}^T gives:

$$\frac{d\underline{m}(\theta)}{d\theta} = - \underline{Q}^T \underline{B} \underline{Q} \underline{m}(\theta) + \underline{Q}^T \underline{S}^* (\theta) \quad (\text{II.35})$$

The operation $\underline{Q}^T \underline{B} \underline{Q}$ on the symmetric matrix \underline{B} is termed a similarity transformation and this diagonalizes the matrix \underline{B} to give a resultant matrix \underline{P} , the diagonal elements of which are the eigenvalues of \underline{B} . In the matrix notation:

$$\underline{Q}^T \underline{B} \underline{Q} = \underline{P} = \begin{bmatrix} p_1 & & & \\ & p_2 & & \\ & & \ddots & \\ & & & p_n \end{bmatrix} \quad (\text{II.36})$$

where p_i ($i = 1$ to n) are the n eigenvalues of \underline{B} .

Also matrices \underline{Q} and \underline{Q}^T are given by (II.37) and (II.38).

$$\underline{Q} = \begin{bmatrix} q_{11} & q_{12} & \dots & q_{1n} \\ q_{21} & \dots & \dots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ q_{n1} & \dots & \dots & q_{nn} \end{bmatrix} \quad (\text{II.37})$$

$$\underline{Q}^T = \begin{bmatrix} q_{11} & q_{21} & \dots & q_{n1} \\ q_{12} & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ q_{1n} & \dots & \dots & q_{nn} \end{bmatrix} \quad (\text{II.38})$$

$$\underline{Q}^T \underline{s}^*(\theta) = \left[\underline{q}_1^T \underline{s}^*(\theta), \underline{q}_2^T \underline{s}^*(\theta), \dots, \underline{q}_n^T \underline{s}^*(\theta) \right] \quad (\text{II.39})$$

Now equation (II.35) becomes:

$$\frac{d\underline{m}(\theta)}{d\theta} = -\underline{P} \underline{m}(\theta) - \underline{Q}^T \underline{s}^*(\theta) \quad (\text{II.40})$$

Each individual equation of the above matrix equation may be put in the following form:

$$\frac{dm_i(\theta)}{d\theta} = -p_i m_i(\theta) + q_j^T \underline{s}^*(\theta) \quad (\text{II.41})$$

The above equation is an ordinary linear differential equation of the first order in one variable $m_i(\theta)$ with the initial condition:

$$m_i(0) = m_{i,0} (= \underline{q}_i^T \underline{u}(0)) \quad (\text{II.42})$$

and can be effectively decoupled from the other variables m_j ($j \neq i$). The equation (II.41) can be integrated to give:

$$m_i(\theta) = e^{-p_i\theta} \left[m_{i,0} + \int_0^\theta e^{p_i\eta} [\underline{q}_i^T \underline{s}^*(\eta)] d\eta \right] \quad (i = 1 \text{ to } n) \quad (\text{II.43})$$

Equation (II.43) is a general solution of equation (II.30).

Rearranging and putting it in compact matrix notation:

$$\begin{bmatrix} m_1(\theta) \\ m_2(\theta) \\ \vdots \\ m_n(\theta) \end{bmatrix} = \begin{bmatrix} e^{-p_1\theta} & & & \\ & e^{-p_2\theta} & & \\ & & \ddots & \\ & & & e^{-p_n\theta} \end{bmatrix} \begin{bmatrix} m_{1,0} \\ m_{2,0} \\ \vdots \\ m_{n,0} \end{bmatrix} + \begin{bmatrix} e^{-p_1\theta} & & & \\ & e^{-p_2\theta} & & \\ & & \ddots & \\ & & & e^{-p_n\theta} \end{bmatrix} \begin{bmatrix} \int_0^\theta e^{p_1\eta} [\underline{q}_1^T \underline{s}^*(\eta)] d\eta \\ \vdots \\ \int_0^\theta e^{p_n\eta} [\underline{q}_n^T \underline{s}^*(\eta)] d\eta \end{bmatrix} \quad (\text{II.44})$$

Premultiplying equation (II.44) by \underline{Q} gives:

$$\begin{bmatrix} u_1(\theta) \\ u_2(\theta) \\ \vdots \\ u_n(\theta) \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & \dots & q_{1n} \\ & q_{21} & & \vdots \\ & \vdots & & \vdots \\ & \vdots & & \vdots \\ q_{n1} & \dots & \dots & q_{nn} \end{bmatrix} \begin{bmatrix} e^{-p_1 \theta} & & & \\ & e^{-p_2 \theta} & & \\ & & \ddots & \\ & & & e^{-p_n \theta} \end{bmatrix} \begin{bmatrix} m_{1,0} \\ m_{2,0} \\ \vdots \\ m_{n,0} \end{bmatrix} + \\
 \begin{bmatrix} q_{11} & q_{12} & & q_{1n} \\ & q_{21} & & \vdots \\ & \vdots & & \vdots \\ & \vdots & & \vdots \\ & \vdots & & \vdots \\ q_{n1} & \dots & \dots & q_{nn} \end{bmatrix} \begin{bmatrix} e^{-p_1 \theta} & & & \\ & e^{-p_2 \theta} & & \\ & & \ddots & \\ & & & e^{-p_n \theta} \end{bmatrix} \begin{bmatrix} \int_0^\theta e^{p_1 \eta} \underline{q}_1^T \underline{s}^*(\eta) d\eta \\ \vdots \\ \int_0^\theta e^{p_n \eta} \underline{q}_n^T \underline{s}^*(\eta) d\eta \end{bmatrix} \quad (\text{II.45})$$

$$\text{But } \underline{m}_0 = \underline{Q}^T \underline{u}_0 \quad (\text{II.46})$$

$$\text{and } \underline{Q}^T \underline{Q} = \underline{I} \quad (\text{II.47})$$

Substitute equation (II.46) in the first term of equation (II.45) and equation (II.47) into the second integral term of equation (II.45) to give:

$$\begin{bmatrix} u_1(\theta) \\ u_2(\theta) \\ \vdots \\ u_n(\theta) \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & \dots & q_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{n1} & \dots & \dots & q_{nn} \end{bmatrix} \begin{bmatrix} e^{-p_1 \theta} \\ e^{-p_2 \theta} \\ \vdots \\ e^{-p_n \theta} \end{bmatrix} \begin{bmatrix} q_{11} & q_{21} & \dots & q_{n1} \\ \vdots & \vdots & \ddots & \vdots \\ q_{1n} & \dots & \dots & q_{nn} \end{bmatrix} \times$$

$$\begin{bmatrix} u_{1,0} \\ u_{2,0} \\ \vdots \\ u_{n,0} \end{bmatrix} + \begin{bmatrix} q_{11} & q_{12} & \dots & q_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{n1} & \dots & \dots & q_{nn} \end{bmatrix} \begin{bmatrix} e^{-p_1 \theta} \\ e^{-p_2 \theta} \\ \vdots \\ e^{-p_n \theta} \end{bmatrix} \times$$

$$\begin{bmatrix} q_{11} & q_{21} & \dots & q_{n1} \\ \vdots & \vdots & \ddots & \vdots \\ q_{1n} & \dots & \dots & q_{nn} \end{bmatrix}^\theta \int_0^\theta \begin{bmatrix} q_{11} & q_{12} & \dots & q_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ q_{n1} & \dots & \dots & q_{nn} \end{bmatrix} \times$$

$$\begin{bmatrix} e^{p_1 \eta} \left[\underline{q}_1^T \underline{s}^*(\eta) \right] d\eta \\ \vdots \\ e^{p_n \eta} \left[\underline{q}_n^T \underline{s}^*(\eta) \right] d\eta \end{bmatrix} \quad (\text{II.48})$$

The following nomenclature is employed:

$$\underline{E}(\theta) = \begin{bmatrix} e^{-p_1 \theta} & & & & \\ & e^{p_2 \theta} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & e^{p_n \theta} \end{bmatrix} \quad (\text{II.49})$$

and

$$\underline{E}^{-1}(\theta) = \begin{bmatrix} e^{p_1 \theta} & & & & \\ & e^{-p_2 \theta} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & e^{-p_n \theta} \end{bmatrix} \quad (\text{II.50})$$

$$\underline{h}(\theta) = \begin{bmatrix} \int_0^\theta e^{p_1 n} \left[\underline{q}_1^T \underline{s}^*(n) \right] d n \\ \vdots \\ \int_0^\theta e^{p_n n} \left[\underline{q}_n^T \underline{s}^*(n) \right] d n \end{bmatrix}$$

$$= \int_0^\theta \begin{bmatrix} e^{p_1 n} \\ e^{p_2 n} \\ \vdots \\ e^{p_n n} \end{bmatrix} \begin{bmatrix} q_{11} & q_{21} & \dots & q_{n1} \\ q_{12} & & & \vdots \\ \vdots & & & \vdots \\ q_{1n} & \dots & \dots & q_{nn} \end{bmatrix} \times$$

$$\begin{bmatrix} s_1^*(n) \\ \vdots \\ s_n^*(n) \end{bmatrix}$$

$d n$

(II.51)

Hence equation (II.48) may be written as:

$$\underline{u}(\theta) = \underline{Q} \underline{E}(\theta) \underline{Q}^T \left[\underline{u}_0 + \int_0^\theta \underline{Q} \underline{E}^{-1}(n) \underline{Q}^T \underline{s}^*(n) dn \right] \quad (\text{II.52})$$

$$\therefore \underline{v}(\theta) = \underline{G}^{*-1/2} \underline{u}(\theta) \quad \text{from equation (II.20)}$$

$$\text{also } \underline{u}_0 = \underline{G}^{*1/2} \underline{v}_0$$

$$\text{and } \underline{s}^*(n) = \underline{G}^{*-1/2} \underline{s}(n)$$

Substituting the values in equation (II.52)

gives:

$$\underline{v}(\theta) = \underline{G}^{*-1/2} \underline{Q} \underline{E}(\theta) \underline{Q}^T \left[\underline{G}^{*1/2} \underline{v}_0 + \int_0^\theta \underline{Q} \underline{E}^{-1}(n) \underline{Q}^T \underline{G}^{*1/2} \underline{s}(n) dn \right]$$

or

$$\underline{v}(\theta) = \underline{G}^{*-1/2} \underline{Q} \underline{E}(\theta) \underline{Q}^T \underline{G}^{*1/2} \left[\underline{v}_0 + \int_0^\theta \underline{G}^{*1/2} \underline{Q} \underline{E}^{-1}(n) \underline{Q}^T \underline{G}^{*-1/2} \underline{s}(n) dn \right] \quad (\text{II.53})$$

Since $\underline{c}(\theta) = \underline{D} \underline{v}(\theta)$ from equation (II.13)

$$\text{also } \underline{v}_0 = \underline{D}^{-1} \underline{c}_0 \text{ and } \underline{s}(n) = \underline{D}^{-1} \underline{s}'(n).$$

Substitution of the above values in the equation

(II.53) gives:

$$\underline{c}(\theta) = \underline{D} \underline{G}^{*-1/2} \underline{Q} \underline{E}(\theta) \underline{Q}^T \underline{G}^{*1/2} \left[\underline{D}^{-1} \underline{c}_0 + \int_0^\theta \underline{G}^{*-1/2} \underline{Q} \underline{E}^{-1}(n) \underline{Q}^T \underline{G}^{*-1/2} \underline{D}^{-1} \underline{s}'(n) dn \right]$$

or

$$\underline{c}(\theta) = \underline{D}\underline{G}^{*-1/2}\underline{Q}\underline{E}(\theta) \underline{Q}^T \underline{G}^{*1/2} \underline{D}^{-1} \left[\underline{c}_0 + \int_0^\theta \underline{D}\underline{G}^{*-1/2} \underline{Q}\underline{E}^{-1}(\eta) \underline{Q}^T \underline{G}^{*-1/2} \underline{D}^{-1} \underline{s}'(\eta) d\eta \right] \quad (\text{II.54})$$

Equation (II.54) represents a general solution of the matrix differential equation, which in turn is the general solution of the dispersion model equation (II.1) or (II.2) after rigorous approximation and discretization of the space derivatives. The integral term may be evaluated analytically if the boundary condition vector $\underline{s}'(\theta)$ is simple; otherwise the numerical integration methods have to be applied.

However, the solution involves the calculation of the eigenvalues and eigenvectors of matrix \underline{B} .

3. Derivation of matrix \underline{D} used for the conversion of the matrix \underline{A}^* to the real, symmetric form.

As discussed earlier matrix \underline{D} is a diagonal matrix, having diagonal elements alternate in sign ie. $d_i = (-1)^i |d_i|$.

The original coefficient matrix \underline{A}^* is converted to a real symmetric matrix using the following similarity transformation.

$$\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D} \quad (\text{II.55})$$

The derivation of the coefficient matrix \underline{A}^* is quite evident from the matrix differential equation (II.28).

For deriving matrix \underline{D} , the actual operation as indicated in equation (II.55) is carried out and a set of equations is derived in terms of the diagonal elements of the matrix \underline{D} so that the final matrix \underline{A} is symmetric. Two sets of equations are given below for one dimensional and two dimensional homogeneous cases. This technique did not work when the coefficient matrix was derived using higher order correct monotone type formulations.

$$\begin{aligned} \frac{d_2}{d_1} &= \frac{d_3}{d_2} = \dots\dots\dots = \frac{d_{i+1}}{d_i} \dots\dots\dots = \frac{d_n}{d_{n-1}} \\ &= \sqrt{\frac{\alpha + \frac{h}{2}}{\alpha - \frac{h}{2}}} \end{aligned} \quad (\text{II.56})$$

The value of d_1 is chosen arbitrarily and the other values are calculated using the above set of equations for one dimensional homogeneous case.

The following sets of equations were derived for two dimensional homogeneous case, thirty point grid,

$$\left[\begin{array}{cccccc}
 \frac{d_2}{d_1} = & \frac{d_3}{d_2} = & \frac{d_4}{d_3} = & \frac{d_5}{d_4} = & & \\
 \frac{d_7}{d_6} = & \frac{d_8}{d_7} = & \frac{d_9}{d_8} = & \frac{d_{10}}{d_9} = & & \\
 \frac{d_{12}}{d_{11}} = & \frac{d_{13}}{d_{12}} = & \frac{d_{14}}{d_{13}} = & \frac{d_{15}}{d_{14}} = & & \\
 \frac{d_{17}}{d_{16}} = & \frac{d_{18}}{d_{17}} = & \frac{d_{19}}{d_{18}} = & \frac{d_{20}}{d_{19}} = & & \\
 \frac{d_{22}}{d_{21}} = & \frac{d_{23}}{d_{22}} = & \frac{d_{24}}{d_{23}} = & \frac{d_{25}}{d_{24}} = & & \\
 \frac{d_{27}}{d_{26}} = & \frac{d_{28}}{d_{27}} = & \frac{d_{29}}{d_{28}} = & \frac{d_{30}}{d_{29}} = & &
 \end{array} \right] = \sqrt{\frac{\alpha + \frac{h}{2}}{\alpha - \frac{h}{2}}} \quad (II.57)$$

$$\left[\begin{array}{cccccc}
 \frac{d_6}{d_1} = & \frac{d_7}{d_2} = & \frac{d_8}{d_3} = & \frac{d_9}{d_4} = & \frac{d_{10}}{d_5} = & k_1 \\
 \frac{d_{11}}{d_6} = & \frac{d_{12}}{d_7} = & \frac{d_{13}}{d_8} = & \frac{d_{14}}{d_9} = & \frac{d_{15}}{d_{10}} = & k_2 \\
 \frac{d_{16}}{d_{11}} = & \frac{d_{17}}{d_{12}} = & \frac{d_{18}}{d_{13}} = & \frac{d_{19}}{d_{14}} = & \frac{d_{20}}{d_{15}} = & k_3 \\
 \frac{d_{21}}{d_{16}} = & \frac{d_{22}}{d_{17}} = & \frac{d_{23}}{d_{18}} = & \frac{d_{24}}{d_{19}} = & \frac{d_{25}}{d_{20}} = & k_4
 \end{array} \right] \quad (II.58)$$

The value of d_1 is chosen arbitrarily and the matrix \underline{D} is derived using the sets of equations represented by (II.57) and (II.58). Then the solution to the forward problem is complete and the various values can be plugged in the equation (II.54) which is the general solution of the dispersion model equation in its semi-discrete form.

III. FORWARD PROBLEM

(SOLUTION OF VARIOUS DISPERSION MODELS)

The solution of the dispersion model equation, (or conductive convective heat transfer (16) or convective diffusion (21) equation for a one dimensional system containing homogeneous, incompressible fluid) transient state problems are presented in this chapter. The coefficient matrices for each of these cases are developed using central difference semi-discrete finite difference approximations. The techniques employed for finding out the eigenvalues and the eigenvectors of the coefficient matrix are discussed in some detail.

A. HOMOGENEOUS MEDIA

1. One Dimensional Case:

(a) Derivation: Consider a tubular reactor of length L through which a fluid is flowing at a constant velocity u . It is also assumed that the fluid is homogeneous, incompressible and the mixing is uniform throughout. The tracer concentration is zero initially. After time zero, the tracer is introduced and the boundary is maintained at this concentration for all the other times. It is required to evaluate the concentration profiles at various elapsed times.

There is no reaction going on inside the reactor and the mixing takes place because of axial dispersion. Consider an elementary section of the reactor as shown in figure III-a.

The basic material balance for the tracer is:

$$\text{Input} + \text{Generation} = \text{Output} + \text{Accumulation} \quad (\text{III.1})$$

$$\begin{aligned} \text{Input} &= (\text{Input})_{\text{Bulk Flow}} + (\text{Input})_{\text{Axial Dispersion}} \\ &= c_{\text{in}} u s + (-D_L s \frac{\partial C}{\partial x})_{\text{in}} \end{aligned} \quad (\text{III.2})$$

$$\begin{aligned} \text{Output} &= (\text{Output})_{\text{Bulk Flow}} + (\text{Output})_{\text{Axial Dispersion}} \\ &= c_{\text{out}} u s + (-D_L s \frac{\partial C}{\partial x})_{\text{out}} \end{aligned} \quad (\text{III.3})$$

$$\text{Accumulation} = s \Delta x \frac{\partial C}{\partial t} \quad (\text{III.4})$$

where s = The cross-sectional area

and t = Time

$$\text{Generation} = 0 \quad (\text{III.5})$$

(\because There is no chemical reaction).

Substitution of (III.2), (III.3), (III.4) and (III.5) in equation (III.1) gives:

$$-D_L s \left(\frac{\partial C}{\partial x} \right)_x + D_L s \left(\frac{\partial C}{\partial x} \right)_{x+\Delta x} + u s (c_{x+\Delta x} - c_x) + s \Delta x \frac{\partial C}{\partial t} = 0$$

or

$$D_L \left[\left(\frac{\partial C}{\partial x} \right)_{x+\Delta x} - \left(\frac{\partial C}{\partial x} \right)_x \right] - u (c_{x+\Delta x} - c_x) = \Delta x \frac{\partial C}{\partial t} \quad (\text{III.6})$$

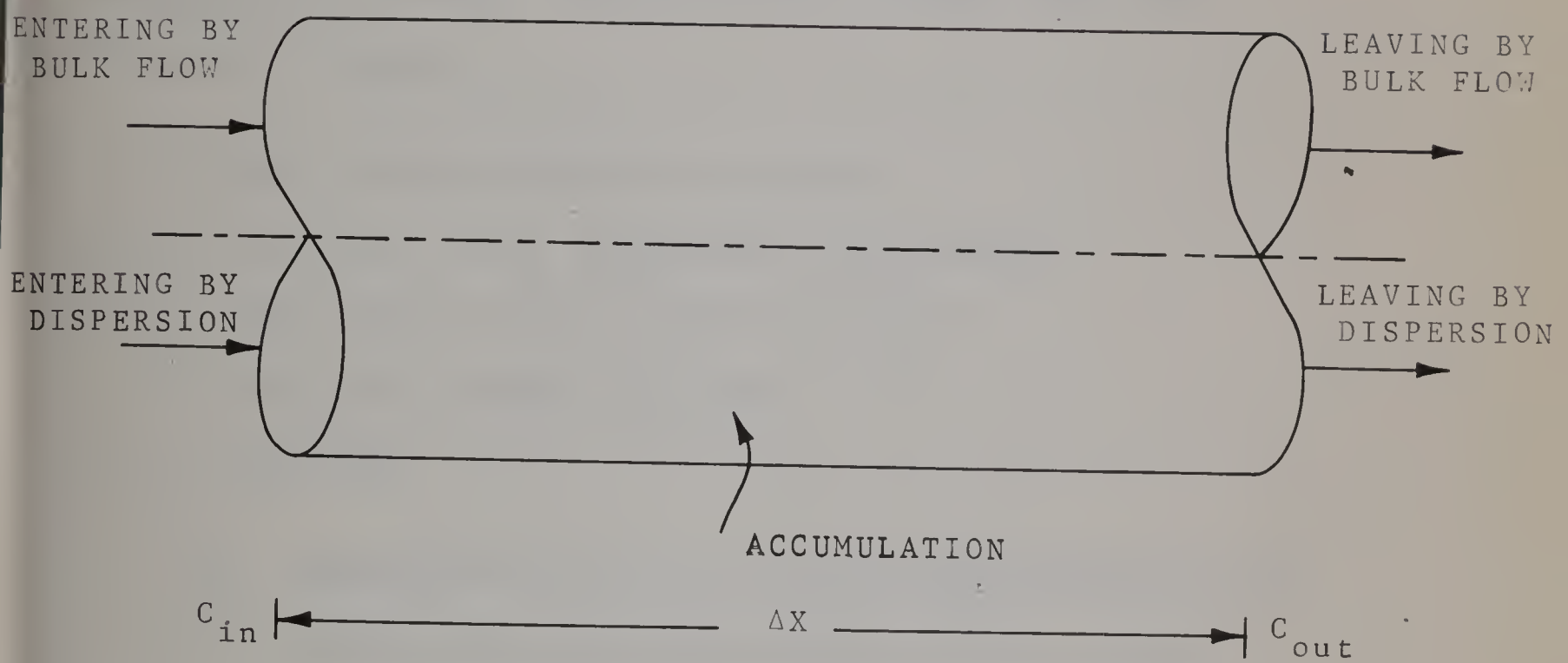


FIGURE III.a MATERIAL BALANCE DIAGRAM ONE DIMENSIONAL
HOMOGENEOUS CASE

Dividing both sides by Δx and approaching the limit as $\Delta x \rightarrow 0$.

$$D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} \quad (\text{III.7})$$

Equation (III.7) describes the one dimensional homogeneous process. The various symbols have the following meaning:

- c = The concentration at any point
- D_L = Effective axial dispersion coefficient
- u = The velocity of the flowing fluid
- x = The axial length variable
- t = The time

(b) Conversion of P.D.E. to the Dimensionless Form:

Define the following dimensionless groups:

$$\left. \begin{aligned} Z &= \frac{x}{L} \quad (\text{Dimensionless Length}) \\ c &= \frac{c}{c_0} \quad (\text{Dimensionless Concentration}) \\ \theta &= \frac{ut}{L} \quad (\text{Reduced Time}) \end{aligned} \right] \quad (\text{III.8})$$

Substitution of (III.8) in (III.7) gives after rearranging:

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial^2 c}{\partial Z^2} - \frac{\partial c}{\partial Z} \quad (\text{III.9})$$

where α = The axial dispersion group and is defined by equation (III.10)

$$\alpha = D_L / uL \quad (\text{III.10})$$

The concentration profiles are evaluated in terms of the dimensionless quantities for a particular value of α .

The equation (III.9) is solved using two sets of boundary conditions given by (III.11) and (III.12).

$$\left. \begin{array}{lll} \text{I.c} & c = 0 & \text{at } \theta = 0 \quad 0 \leq z \leq 1 \\ \text{B.c} & c = 1 & \text{at } z = 0 \quad \theta > 0 \\ & \frac{\partial c}{\partial z} = 0 & \text{at } z = 1 \end{array} \right] \quad (\text{III.11})$$

The above set is termed as the ordinary boundary conditions in this work.

$$\left. \begin{array}{lll} \text{I.c} & c = 0 & \text{at } \theta = 0 \quad 0 \leq z \leq 1 \\ \text{B.c} & c_{z \rightarrow 0+} - \alpha \left(\frac{\partial c}{\partial z} \right)_{z \rightarrow 0+} = 1, & \text{at } z = 0, \theta > 0 \\ & \frac{\partial c}{\partial z} = 0 & \text{at } z = 1 \end{array} \right] \quad (\text{III.12})$$

The above set is termed as

Danckwerts boundary conditions (8).

The analytical solution to the equation (III.9) with these sets of boundary conditions (III.11) and (III.12) is not available, however, corresponding to some other sets

TABLE III.1

One dimensional Homogeneous Case: (Using Ordinary Boundary Conditions)

Summary of Results*: Comparison of Ten-point Grid.

(The results of a ten-point grid are derived from those of a twenty point grid using interpolation and compared with the generated values using the semi-analytical technique).

A complete set of results is available in

Appendix B.

Grid Point Reduced Time θ	1	3	5	7	9
0.2	0.88133 0.88238 0.00105	0.55646 0.55860 0.00214	0.25744 0.25543 -0.00200	0.08665 0.08168 -0.00497	0.02199 0.01838 -0.00361
0.4	0.95032 0.95000 -0.00032	0.79125 0.79118 -0.00007	0.57632 0.57668 0.00036	0.36106 0.36034 -0.00072	0.20270 0.20030 -0.00240
0.6	0.97425 0.97348 -0.00077	0.88695 0.88522 -0.00173	0.75191 0.75040 -0.00151	0.58862 0.58780 -0.00082	0.44237 0.44237 0.00000
0.8	0.98543 0.98447 -0.00096	0.93458 0.93196 -0.00262	0.85080 0.84771 -0.00309	0.74126 0.73886 -0.00240	0.63584 0.63501 -0.00083
1.0	0.99144 0.99040 -0.00104	0.96104 0.95794 -0.00310	0.90924 0.90505 -0.00419	0.83905 0.83494 -0.00411	0.76945 0.76645 -0.00300

* The first entry in each block refers to the value of c calculated using semi-analytical technique; the second entry refers to the interpolated value; the third entry represents the deviation. Interpolated value - the value calculated by semi-analytical solution.

TABLE III.2

One dimensional Homogeneous Case: (Using Danckwerts Boundary Conditions).

Summary of Results*: Ten-point grid comparison.

(The results of a ten-point grid are derived from those of a twenty point grid using interpolation and compared with the generated values using semi-analytical technique).

Grid Point Reduced Time θ	1	3	5	7	9
0.2	0.59343 0.58629 -0.00714	0.32805 0.31648 -0.01157	0.13632 0.12557 -0.01075	0.04224 0.03561 -0.00663	0.01006 0.00724 -0.00282
0.4	0.77676 0.76656 -0.00020	0.58441 0.58037 -0.00404	0.39046 0.38371 -0.00675	0.22585 0.21805 -0.0078	0.11784 0.11055 -0.00729
0.6	0.85480 0.85543 0.00063	0.73273 0.73097 -0.00176	0.58225 0.57835 -0.0039	0.42668 0.42118 -0.0055	0.30100 0.29491 -0.00609
0.8	0.90586 0.90581 -0.00005	0.82367 0.82190 -0.00177	0.71444 0.71122 -0.00322	0.59074 0.58652 -0.00422	0.48196 0.47756 -0.0044
1.0	0.93756 0.93651 -0.00105	0.88193 0.87936 -0.00257	0.80481 0.80112 -0.00369	0.71329 0.70904 -0.00425	0.62955 0.62548 -0.00407

* The first entry in each block refers to the value of c calculated using semi-analytical solution; the second entry refers to the interpolated value; the third entry refers to the deviation: Interpolated value - the value calculated by semi-analytical solution.

A complete set of results is available in Appendix B.

of boundary conditions the analytical solutions are available in (4, 17). Therefore the accuracy of the solution is tested by comparing the results of different grid spacings. The summarised results are represented in tables (III.1) and (III.2) for both sets of boundary conditions.

Ten point grid and twenty point grid are used to obtain a general solution. The distance ($0 \leq z \leq 1$) is divided into a finite number of grid points of width h , with a slab of width $\frac{h}{2}$ near the boundary where the boundary condition is specified (Fig. III-b). By replacing the space derivatives with the central difference semi discrete finite difference formulations, the following ordinary matrix differential equation is obtained.

$$\frac{d}{d\theta} \begin{bmatrix} w_1 \\ w_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ w_{10} \end{bmatrix} = -\frac{1}{h^2} \begin{bmatrix} 0.4 & -0.1091 & & & & & \\ -0.2909 & 0.4 & -0.1091 & & & & \\ & \dots & \dots & \dots & \dots & & \\ & & \dots & \dots & \dots & & \\ & & & -0.2909 & 0.4 & -0.1091 & \\ & & & & -0.2909 & 0.2909 & \end{bmatrix}$$

$$\begin{bmatrix} w_1 \\ w_2 \\ \cdot \\ \cdot \\ w_{10} \end{bmatrix} + \frac{1}{h^2} \begin{bmatrix} 0.2909 \\ 0 \\ \cdot \\ \cdot \\ 0 \end{bmatrix} \quad (III.13)$$

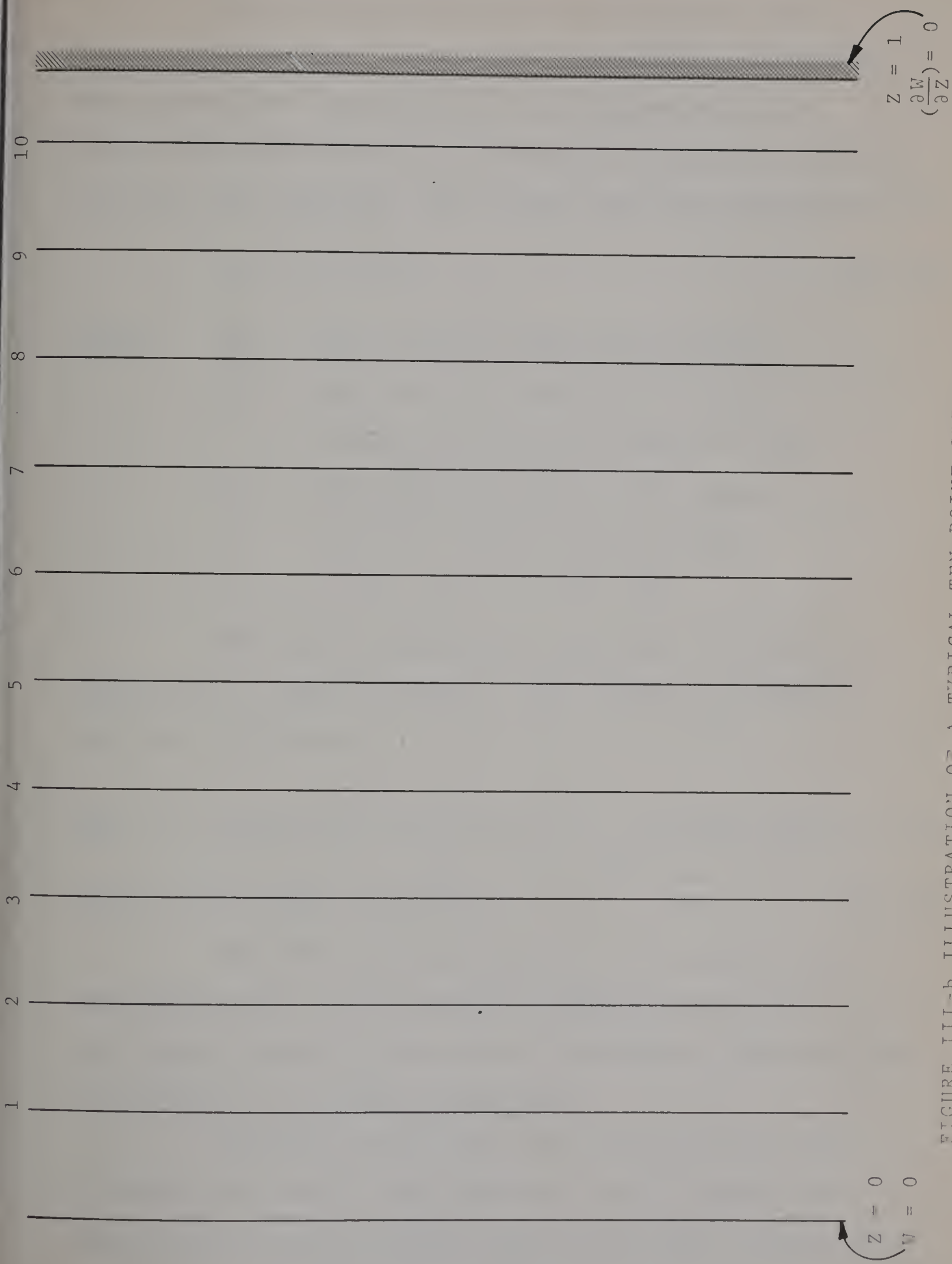


FIGURE III-6 ILLUSTRATION OF A TYPICAL TEN POINT GRID
ONE DIMENSIONAL HOMOGENEOUS CASE

The coefficient matrix is unsymmetric and diagonally dominant. To use the conventional techniques for finding out the eigenvalues and eigenvectors of a real symmetric matrix, the resultant matrix is converted into the real symmetric form using similarity transformation

$$\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D} \quad (\text{III.14})$$

where \underline{A}^* = the original coefficient matrix
 \underline{A} = the original coefficient matrix
converted into real symmetric form
 \underline{D} = the diagonal matrix with diagonal
entries having alternate signs

$$\text{i.e. } d_i = (-1)^i |d_i|$$

The above technique is discussed in detail in Chapter II of general theory. The solution of equation (III.13) is given by

$$\underline{W}(\theta) = \underline{D} \underline{Q} \underline{E}(\theta) \underline{Q}^T \underline{D}^{-1} \left[\underline{W}^{(0)}(\theta) + \int_0^\theta \underline{D} \underline{Q} \underline{E}^{-1}(\eta) \underline{Q}^T \underline{D}^{-1} \underline{s}'(\eta) d\eta \right]$$

where η is a dummy variable. (III.15)

For this particular case of a ten point grid the matrices \underline{A}^* , \underline{A} , the matrix of eigenvectors \underline{Q} and the diagonal matrix \underline{D} are given in appendix B corresponding to both sets of boundary conditions.

Appendix B also gives the above matrices for a twenty point grid. The values of the ten point grid derived from those of twenty point grid using interpolation

are compared with the corresponding values obtained by using the semi-analytical solution and the check for their closeness is made. The results are given in appendix B in detail.

2. Two Dimensional Case:

(a) Derivation: In this case the mixing takes place both by axial dispersion as well as by radial dispersion. Consider an elementary section of the reactor as given in figure III-c. The rest of the problem is essentially the same as in the one dimensional case.

The basic material balance is given by equation (III.1).

$$\begin{aligned}
 \text{Input} &= (\text{Input})_{\text{Bulk Flow}} + (\text{Input})_{\text{Axial Dispersion}} \\
 &\quad + (\text{Input})_{\text{Radial Dispersion}} \\
 &= u2\pi r\Delta r c_x + (-D_L 2\pi r\Delta r \frac{\partial c}{\partial x})_x + (-D_R 2\pi r\Delta x \frac{\partial c}{\partial r})_r \quad (\text{III.16})
 \end{aligned}$$

$$\begin{aligned}
 \text{Output} &= (\text{Output})_{\text{Bulk Flow}} + (\text{Output})_{\text{Axial Dispersion}} \\
 &\quad + (\text{Output})_{\text{Radial Dispersion}} \\
 &= u2\pi r\Delta r c_{x+\Delta x} + (-D_L 2\pi r\Delta r \frac{\partial c}{\partial x})_{x+\Delta x} \\
 &\quad + (-D_R 2\pi r\Delta x \frac{\partial c}{\partial r})_{r+\Delta r} \quad (\text{III.17})
 \end{aligned}$$

$$\text{Generation} = 0 \quad (\text{III.18})$$

$$\text{Accumulation} = 2\pi r\Delta r\Delta x \frac{\partial c}{\partial t} \quad (\text{III.19})$$

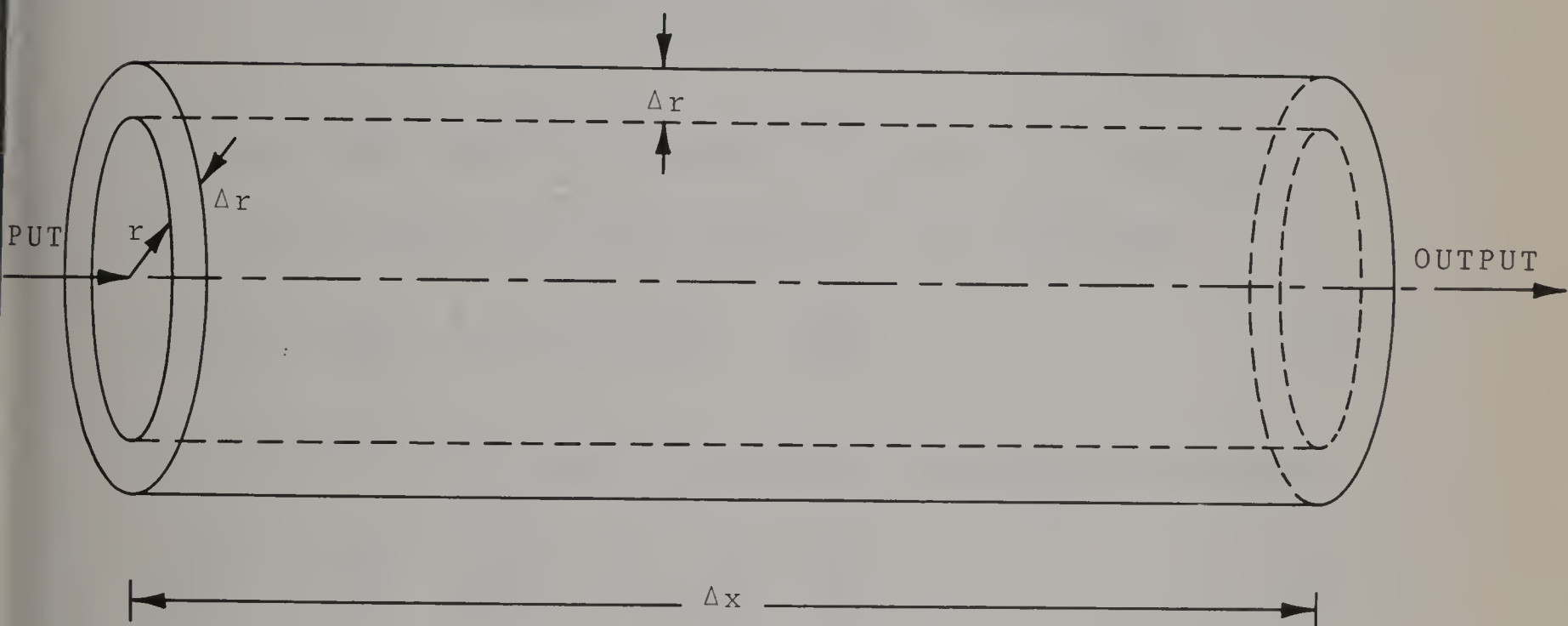


FIGURE III-c MATERIAL BALANCE DIAGRAM TWO DIMENSIONAL
HOMOGENEOUS CASE

Substituting equations (III.16) through (III.19) in the basic material balance equation and rearranging

$$D_L 2\pi r \Delta r \left[\left(\frac{\partial C}{\partial x} \right)_{x+\Delta x} - \left(\frac{\partial C}{\partial x} \right)_x \right] + D_R 2\pi r \Delta x \left[\left(r \frac{\partial C}{\partial r} \right)_{r+\Delta r} - \left(r \frac{\partial C}{\partial r} \right)_r \right] = u 2\pi r \Delta r \left[C_{x+\Delta x} - C_x \right] + 2\pi r \Delta r \Delta x \frac{\partial C}{\partial t} \quad (\text{III.20})$$

Dividing both sides of equation (III.20) by $(2\pi r \Delta r \Delta x)$ and approaching the limit as $\Delta x, \Delta r \rightarrow 0$, one gets:

$$D_L \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} + \frac{1}{r} D_R \frac{\partial}{\partial r} \left(r \frac{\partial C}{\partial r} \right) = \frac{\partial C}{\partial t} \quad (\text{III.21})$$

Upon expanding the term in brackets the equation becomes:

$$D_L \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} + D_R \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} D_R \frac{\partial C}{\partial r} = \frac{\partial C}{\partial t} \quad (\text{III.22})$$

Hence equation (III.21) or (III.22) represents the two dimensional homogeneous case.

(b) Conversion of P.D.E. to the Dimensionless Form:

As in the one dimensional case define the following dimensionless quantities:

$$\begin{aligned}
 c &= \frac{c}{c_0} \quad (\text{Dimensionless Concentration}) \\
 z &= \frac{x}{L} \quad (\text{Dimensionless length}) \\
 &\quad \text{i.e. axial variable} \\
 R &= \frac{r}{R_0} \quad (\text{Dimensionless Radial Variable}) \\
 &\quad \text{where } R_0 = \text{The radius of the} \\
 &\quad \text{tubular reactor.} \\
 \alpha &= \frac{D_L}{UL} \quad (\text{Axial dispersion group}) \\
 \beta &= \frac{D_R}{uR_0} \quad (\text{Radial dispersion group}) \\
 \theta &= \frac{ut}{L} \quad (\text{Reduced time}) \\
 \gamma &= \frac{L}{R_0} \quad (\text{Constant})
 \end{aligned}
 \tag{III.23}$$

Substituting the values of the dimensionless groups in equation (III.22) and rearranging we get:

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} + \beta \gamma \frac{\partial^2 c}{\partial R^2} + \frac{1}{R} \beta \gamma \frac{\partial c}{\partial R}
 \tag{III.24}$$

\therefore The value of $\frac{1}{R} \frac{\partial c}{\partial R}$ is indeterminate at the centre.

\therefore A special equation can be derived which is applicable at the centre only.

Differentiating the numerator and the denominator as indicated w.r.t. R:

$$\frac{1}{R} \frac{\partial C}{\partial R} = \frac{\frac{\partial}{\partial R} \left(\frac{\partial C}{\partial R} \right)}{\frac{\partial}{\partial R} (R)} = \frac{\partial^2 C}{\partial R^2} \quad (\text{III.25})$$

Substitution of equation (III.25) in (III.24) gives:

$$\frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} + 2\beta\gamma \frac{\partial^2 C}{\partial R^2} \quad (\text{III.26})$$

The concentration profiles are evaluated in terms of the dimensionless quantities using average values of α and β . Equation (III.24) along with (III.26) is solved using two sets of boundary conditions as given by (III.27) and (III.28).

ORDINARY BOUNDARY CONDITIONS

$$\text{I.c} \quad c = 0 \quad \text{at} \quad \theta = 0 \quad 0 \leq z \leq 1$$

$$\text{B.c} \quad c = 1 \quad \text{at} \quad z = 0 \quad \theta > 0$$

$$\frac{\partial C}{\partial z} = 0 \quad \text{at} \quad z = 1$$

$$\frac{\partial C}{\partial R} = 0 \quad \text{at} \quad R = 0 \quad (\text{Radial Symmetry})$$

$$\frac{\partial C}{\partial R} = 0 \quad \text{at} \quad R = 1 \quad (\text{No flow across the boundary})$$

(III.27)

DANCKWERTS BOUNDARY CONDITIONS

$$\begin{array}{lcl}
 \text{I.c} & c = 0 & \text{at } \theta = 0 \\
 \text{B.c} & c_{z \rightarrow 0+} - \alpha \left(\frac{\partial c}{\partial z} \right)_{z \rightarrow 0+} = 1 & \text{at } z = 0 \\
 & \frac{\partial c}{\partial z} = 0 & \text{at } z = 1 \\
 & \frac{\partial c}{\partial R} = 0 & \text{at } R = 0 \\
 & \frac{\partial c}{\partial R} = 0 & \text{at } R = 1
 \end{array} \quad (III.28)$$

In this case the solution for the upper half of the reactor was obtained because the solution for the lower half is the same taking into account the radial symmetry.

The finite difference grid is shown in the figure III-d. The partial differential equation (III.24) can be approximated to a set of ordinary differential equations using a central difference semi-discrete finite difference approximations, which may be written as:

$$\frac{dc_1}{d\theta} = \frac{1}{h^2} \left[-2(\alpha + 8\beta) c_1 + (\alpha - \frac{h}{2}) c_2 + 16\beta c_6 \right] + \frac{1}{h^2} (\alpha + \frac{h}{2}) \quad (III.29.1)$$

$$\frac{dc_2}{d\theta} = \frac{1}{h^2} \left[(\alpha + \frac{h}{2}) c_1 - 2(\alpha + 8\beta) c_2 + (\alpha - \frac{h}{2}) c_3 + 16\beta c_7 \right] \quad (III.29.2)$$

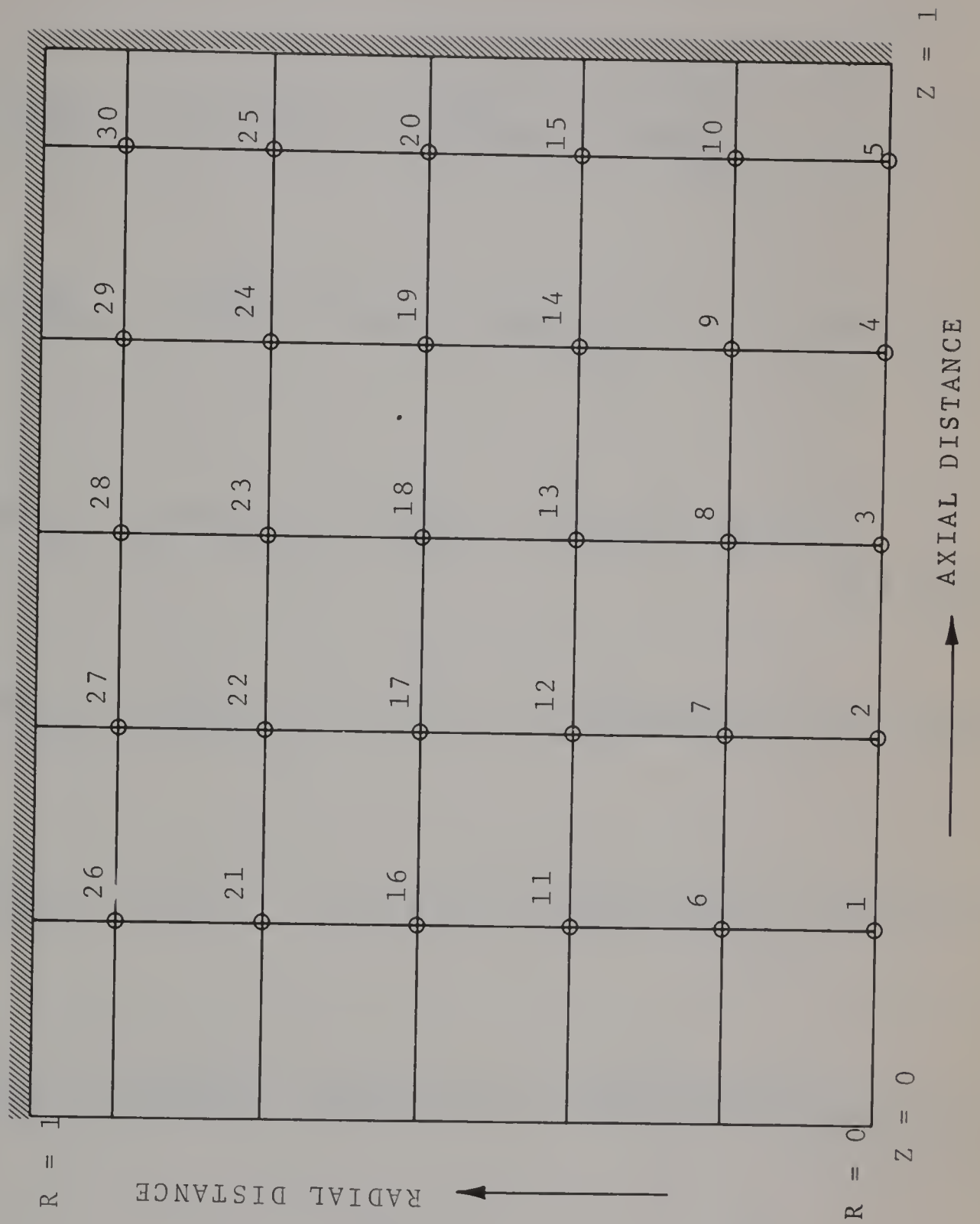


FIGURE III-d TWO DIMENSIONAL HOMOGENEOUS CASE

$$\frac{dc_3}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_2 - 2(\alpha + 8\beta) c_3 + \left(\alpha - \frac{h}{2}\right) c_4 + 16\beta c_8 \right] \quad (\text{III.29.3})$$

$$\frac{dc_4}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_3 - 2(\alpha + 8\beta) c_4 + \left(\alpha - \frac{h}{2}\right) c_5 + 16\beta c_9 \right] \quad (\text{III.29.4})$$

$$\frac{dc_5}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2}\right) c_4 - 2\left(\frac{\alpha + \frac{h}{2}}{2} + 8\beta\right) c_5 + 16\beta c_{10} \right] \quad (\text{III.29.5})$$

$$\frac{dc_6}{d\theta} = \frac{1}{h^2} \left[2\beta c_1 - 2(\alpha + 4\beta) c_6 + \left(\alpha - \frac{h}{2}\right) c_7 + 6\beta c_{11} \right] + \frac{1}{h^2} \left(\alpha + \frac{h}{2}\right) \quad (\text{III.29.6})$$

$$\frac{dc_7}{d\theta} = \frac{1}{h^2} \left[2\beta c_2 + \left(\alpha + \frac{h}{2}\right) c_6 - 2(\alpha + 4\beta) c_7 + \left(\alpha - \frac{h}{2}\right) c_8 + 6\beta c_{12} \right] \quad (\text{III.29.7})$$

$$\frac{dc_8}{d\theta} = \frac{1}{h^2} \left[2\beta c_3 + \left(\alpha + \frac{h}{2}\right) c_7 - 2(\alpha + 4\beta) c_8 + \left(\alpha - \frac{h}{2}\right) c_9 + 6\beta c_{13} \right] \quad (\text{III.29.8})$$

$$\frac{dc_9}{d\theta} = \frac{1}{h^2} \left[2\beta c_4 + \left(\alpha + \frac{h}{2}\right) c_8 - 2(\alpha + 4\beta) c_9 + \left(\alpha - \frac{h}{2}\right) c_{10} + 6\beta c_{14} \right] \quad (\text{III.29.9})$$

$$\frac{dc_{10}}{d\theta} = \frac{1}{h^2} \left[2\beta c_5 + \left(\alpha + \frac{h}{2}\right) c_9 - 2\left(\frac{\alpha + \frac{h}{2}}{2} + 4\beta\right) c_{10} + 6\beta c_{15} \right] \quad (\text{III.29.10})$$

$$\frac{dc_{11}}{d\theta} = \frac{1}{h^2} \left[3\beta c_6 - 2(\alpha + 4\beta) c_{11} + (\alpha - \frac{h}{2}) c_{12} + 5\beta c_{16} \right] + \frac{1}{h^2} (\alpha + \frac{h}{2})$$

(III.29.11)

$$\frac{dc_{12}}{d\theta} = \frac{1}{h^2} \left[3\beta c_7 + (\alpha + \frac{h}{2}) c_{11} - 2(\alpha + 4\beta) c_{12} + (\alpha - \frac{h}{2}) c_{13} + 5\beta c_{17} \right]$$

(III.29.12)

$$\frac{dc_{13}}{d\theta} = \frac{1}{h^2} \left[3\beta c_8 + (\alpha + \frac{h}{2}) c_{12} - 2(\alpha + 4\beta) c_{13} + (\alpha - \frac{h}{2}) c_{14} + 5\beta c_{18} \right]$$

(III.29.13)

$$\frac{dc_{14}}{d\theta} = \frac{1}{h^2} \left[3\beta c_9 + (\alpha + \frac{h}{2}) c_{13} - 2(\alpha + 4\beta) c_{14} + (\alpha - \frac{h}{2}) c_{15} + 5\beta c_{19} \right]$$

(III.29.14)

$$\frac{dc_{15}}{d\theta} = \frac{1}{h^2} \left[3\beta c_{10} + (\alpha + \frac{h}{2}) c_{14} - 2(\frac{\alpha + \frac{h}{2}}{2} + 4\beta) c_{15} + 5\beta c_{20} \right]$$

(III.29.15)

$$\frac{dc_{16}}{d\theta} = \frac{1}{h^2} \left[\frac{10\beta}{3} c_{11} - 2(\alpha + 4\beta) c_{16} + (\alpha - \frac{h}{2}) c_{17} + \frac{14\beta}{3} c_{21} \right] + \frac{1}{h^2} (\alpha + \frac{h}{2})$$

(III.29.16)

$$\frac{dc_{17}}{d\theta} = \frac{1}{h^2} \left[\frac{10\beta}{3} c_{12} + (\alpha + \frac{h}{2}) c_{16} - 2(\alpha + 4\beta) c_{17} + (\alpha - \frac{h}{2}) c_{18} + \frac{14\beta}{3} c_{22} \right]$$

(III.29.17)

$$\frac{dc_{18}}{d\theta} = \frac{1}{h^2} \left[\frac{10\beta}{3} c_{13} + (\alpha + \frac{h}{2}) c_{17} - 2(\alpha + 4\beta) c_{18} + (\alpha - \frac{h}{2}) c_{19} + \frac{14\beta}{3} c_{23} \right]$$

(III.29.18)

$$\frac{dc_{19}}{d\theta} = \frac{1}{h^2} \left[\frac{10}{3} \beta c_{14} + \left(\alpha + \frac{h}{2}\right) c_{18} - 2(\alpha + 4\beta) c_{19} + \left(\alpha - \frac{h}{2}\right) c_{20} + \frac{14}{3} \beta c_{24} \right] \quad (\text{III.29.19})$$

$$\frac{dc_{20}}{d\theta} = \frac{1}{h^2} \left[\frac{10}{3} \beta c_{15} + \left(\alpha + \frac{h}{2}\right) c_{19} - 2\left(\frac{\alpha + \frac{h}{2}}{2} + 4\beta\right) c_{20} + \frac{14}{3} \beta c_{25} \right] \quad (\text{III.29.20})$$

$$\frac{dc_{21}}{d\theta} = \frac{1}{h^2} \left[\frac{7}{2} \beta c_{16} - 2(\alpha + 4\beta) c_{21} + \left(\alpha - \frac{h}{2}\right) c_{22} + \frac{9}{2} \beta c_{26} \right] + \frac{1}{h^2} \left(\alpha + \frac{h}{2}\right) \quad (\text{III.29.21})$$

$$\frac{dc_{22}}{d\theta} = \frac{1}{h^2} \left[\frac{7}{2} \beta c_{17} + \left(\alpha + \frac{h}{2}\right) c_{21} - 2(\alpha + 4\beta) c_{22} + \left(\alpha - \frac{h}{2}\right) c_{23} + \frac{9}{2} \beta c_{27} \right] \quad (\text{III.29.22})$$

$$\frac{dc_{23}}{d\theta} = \frac{1}{h^2} \left[\frac{7}{2} \beta c_{18} + \left(\alpha + \frac{h}{2}\right) c_{22} - 2(\alpha + 4\beta) c_{23} + \left(\alpha - \frac{h}{2}\right) c_{24} + \frac{9}{2} \beta c_{28} \right] \quad (\text{III.29.23})$$

$$\frac{dc_{24}}{d\theta} = \frac{1}{h^2} \left[\frac{7}{2} \beta c_{19} + \left(\alpha + \frac{h}{2}\right) c_{23} - 2(\alpha + 4\beta) c_{24} + \left(\alpha - \frac{h}{2}\right) c_{25} + \frac{9}{2} \beta c_{29} \right] \quad (\text{III.29.24})$$

$$\frac{dc_{25}}{d\theta} = \frac{1}{h^2} \left[\frac{7}{2} \beta c_{20} + \left(\alpha + \frac{h}{2}\right) c_{24} - 2\left(\frac{\alpha + \frac{h}{2}}{2} + 4\beta\right) c_{25} + \frac{9}{2} \beta c_{30} \right] \quad (\text{III.29.25})$$

$$\frac{dc_{26}}{d\theta} = \frac{1}{h^2} \left[\frac{18}{5} \beta c_{21} - (2\alpha + \frac{18}{5}\beta) c_{26} + (\alpha - \frac{h}{2}) c_{27} \right] + \frac{1}{h^2} (\alpha + \frac{h}{2}) \quad (\text{III.29.26})$$

$$\frac{dc_{27}}{d\theta} = \frac{1}{h^2} \left[\frac{18}{5} \beta c_{22} + (\alpha + \frac{h}{2}) c_{26} - (2\alpha + \frac{18}{5}\beta) c_{27} + (\alpha - \frac{h}{2}) c_{28} \right] \quad (\text{III.29.27})$$

$$\frac{dc_{28}}{d\theta} = \frac{1}{h^2} \left[\frac{18}{5} \beta c_{23} + (\alpha + \frac{h}{2}) c_{27} - (2\alpha + \frac{18}{5}\beta) c_{28} + (\alpha - \frac{h}{2}) c_{29} \right] \quad (\text{III.29.28})$$

$$\frac{dc_{29}}{d\theta} = \frac{1}{h^2} \left[\frac{18}{5} \beta c_{24} + (\alpha + \frac{h}{2}) c_{28} - (2\alpha + \frac{18}{5}\beta) c_{29} + (\alpha - \frac{h}{2}) c_{30} \right] \quad (\text{III.29.29})$$

$$\frac{dc_{30}}{d\theta} = \frac{1}{h^2} \left[\frac{18}{5} \beta c_{25} + (\alpha + \frac{h}{2}) c_{29} - (\alpha + \frac{h}{2} + \frac{18}{5}\beta) c_{30} \right] \quad (\text{III.29.30})$$

The above set of equations (III.29.1) through (III.29.30) is obtained by the substitution of the following expressions for the space derivatives at these grid points and using ordinary boundary conditions.

$$\left. \begin{aligned} \frac{\partial^2 c}{\partial z^2} &= \frac{c_{i+1,j} - 2c_{i,j} + c_{i-1,j}}{h^2} \\ \frac{\partial c}{\partial z} &= \frac{c_{i+1,j} - c_{i-1,j}}{2h} \\ \frac{\partial^2 c}{\partial R^2} &= \frac{c_{i,j+1} - 2c_{i,j} + c_{i,j-1}}{k^2} \\ \frac{\partial c}{\partial R} &= \frac{c_{i,j+1} - c_{i,j-1}}{2k} \end{aligned} \right] \quad (\text{III.30})$$

where the subscript i refers to the axial variable
and j to the radial variable and

h = The grid spacing along the axial distance

k = The grid spacing along the radial distance.

The value of γ is taken as 4 in the set of
ordinary differential equations defined by (III.29.1) through
(III.29.30).

The nomenclature of equations represented by
(III.30) can become clear by referring to figure III-e.

The set of ordinary differential equations
(III.29.1) through (III.29.30) may be written in terms
of the following matrix differential equation:

$$\frac{d\underline{w}(\theta)}{d\theta} = - \underline{A}^* \underline{w}(\theta) + \underline{s}'(\theta) \quad (\text{III.31})$$

where

\underline{A}^* = The original coefficient matrix
 $\underline{s}'(\theta)$ = The boundary condition vector
 $\underline{w}(\theta)$ = The vector of unknowns

The solution of the above matrix differential
equation is discussed in detail in Chapter II of General
Theory.

The matrix \underline{A}^* as it appears in the matrix
differential equation (III.31) is converted to the real
symmetric matrix \underline{A} using the same kind of similarity

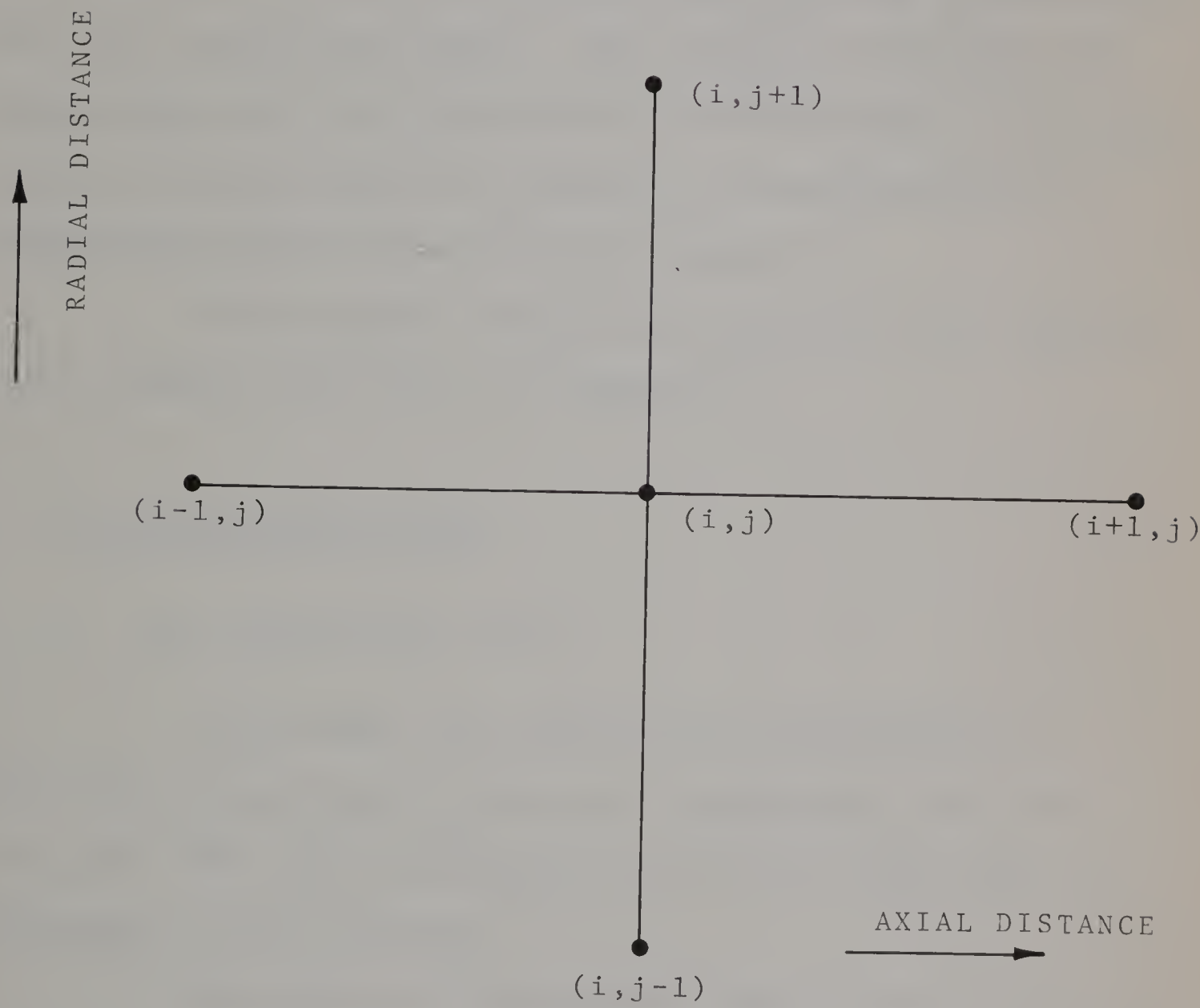


FIGURE III-e NOMENCLATURE DIAGRAM FOR (III.30)

transformation as in the one dimensional homogeneous case i.e. $\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D}$ where the matrices \underline{A} , \underline{A}^* and \underline{D} are given in Appendix C. A thirty point grid was chosen and the results corresponding to both sets of boundary conditions are presented in Appendix C. No analytical solution is available to the partial differential equation representing this two dimensional model. The accuracy with which the eigenvalues and the eigenvectors are determined is clearly evident from the check of similarity transformation to produce the matrix \underline{A} as given in Appendix C.

The relevant computer programs and the complete set of results are given in Appendix C.

B. Non Homogeneous Media

1. One Dimensional Case:

This takes into account the dependency of the media properties on the space position, but not the time. The semi-analytical solution for this case is presented in this section.

The partial differential equation describing the overall process is:

$$\frac{\partial c}{\partial \theta} = \frac{1}{uL} \frac{\partial}{\partial z} \left(D_L \frac{\partial c}{\partial z} \right) - \frac{\partial c}{\partial z} \quad (\text{III.32})$$

where u = The velocity of the flowing fluid and is assumed as constant.

L = The characteristic length of the reactor.

D_L = The axial dispersion coefficient which is assumed as a linear function of z .

$$\text{i.e. } D_L = a + bz = f(z)$$

where a and b are constants.

The equation (III.32) is solved using the following sets of boundary conditions:

$$\left. \begin{array}{l} \text{I.c} \quad c = 0 \quad \text{at} \quad \theta = 0 \quad 0 \leq z \leq 1 \\ \text{B.c} \quad c = 1 \quad \text{at} \quad z = 0 \quad \theta > 0 \\ \frac{\partial c}{\partial z} = 0 \quad \text{at} \quad z = 1 \end{array} \right] \quad (\text{III.33})$$

and

$$\left. \begin{array}{l} \text{I.c} \quad c = 0 \quad \text{at} \quad \theta = 0 \quad 0 \leq z \leq 1 \\ c_{z \rightarrow 0^+} - \frac{1}{uL} (D_L \frac{\partial c}{\partial z})_{z \rightarrow 0^+} = 1 \quad \text{at} \quad z = 0 \quad \theta > 0 \\ \frac{\partial c}{\partial z} = 0 \quad \text{at} \quad z = 1 \end{array} \right] \quad (\text{III.34})$$

A finite difference grid is considered and the length $0 \leq z \leq 1$ is divided into a finite number of increments (n) of width h each, with a slab of width $h/2$ near the boundary where the boundary conditions is specified. The grid is shown in figure III-f.

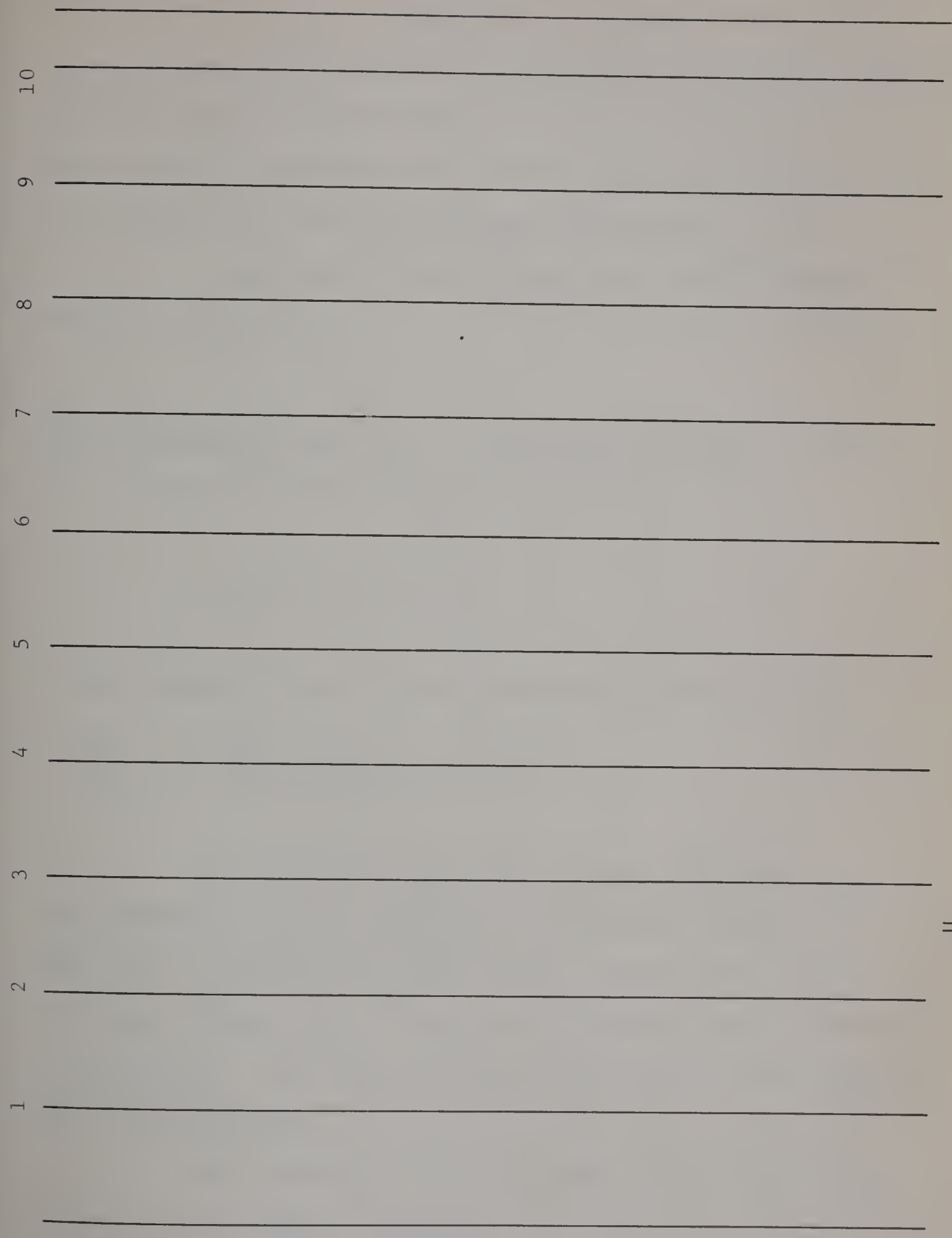


FIGURE III-f

TYPICAL GRID SPACING ONE DIMENSIONAL NON-HOMOGENEOUS CASE

If the axial dispersion coefficient (or the diffusivity) may be represented by discrete values for each of these grid points, the partial differential equation (III.32) can be transformed to a set of ordinary differential equations by discretization of the space derivatives using an appropriate finite difference formulation.

Consider the mass balance on the i^{th} element which is given by:

$$\frac{dc_i}{d\theta} = \frac{(D_L)_{i+1/2} (c_{i+1} - c_i)}{h} - \frac{(D_L)_{i-1/2} (c_i - c_{i-1})}{h} \quad (\text{III.35})$$

for $(i = 1, (n-1))$

\therefore The value of the flux is specified at the boundary.

$$\therefore \frac{dc_n}{d\theta} = \frac{(D_L)_{n-1/2} (c_{i-1} - c_i)}{h^2} \quad (\text{III.36})$$

In the equations (III.35) and (III.36) the effective axial dispersion coefficient between i^{th} and $(i+1)^{\text{th}}$ element is taken as that value for a point half way between the i^{th} and $(i+1)^{\text{th}}$ planes and is denoted by $(D_L)_{i+1/2}$. This approximation is valid if the function $f(z)$ is continuous.

The equations (III.35) and (III.36) may be put in the matrix form as follows:

$$\frac{d}{d\theta} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_n \end{bmatrix} = -\frac{1}{h^2} \begin{bmatrix} k \left[(D_L)_{1/2} + (D_L)_{3/2} \right] & - \left[k (D_L)_{3/2} - \frac{h}{2} \right] \\ -k \left[k (D_L)_{3/2} + \frac{h}{2} \right] & k \left[(D_L)_{3/2} + (D_L)_{5/2} \right] - \left[k (D_L)_{5/2} - \frac{h}{2} \right] \\ \dots & \dots \\ - \left[k (D_L)_{n-3/2} + \frac{h}{2} \right] & k \left[(D_L)_{n-3/2} + (D_L)_{n-1/2} \right] \\ & - k (D_L)_{n-1/2} - \frac{h}{2} - k (D_L)_{n-1/2} \\ & k (D_L)_{n-1/2} & k (D_L)_{n-1/2} \end{bmatrix}$$

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ c_n \end{bmatrix} + \frac{1}{h^2} \begin{bmatrix} \left[k (D_L)_{1/2} + \frac{h}{2} \right] \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 0 \end{bmatrix} \quad (III.37)$$

According to the equation (III.31) the various matrices can be designated as:

$$\underline{A}^* = \begin{bmatrix} k \left[(D_L)_{1/2} + (D_L)_{3/2} \right] & - \left[k (D_L)_{1/2} - \frac{h}{2} \right] \\ - \left[k (D_L)_{3/2} + \frac{h}{2} \right] & k \left[(D_L)_{3/2} + (D_L)_{5/2} \right] - \left[k (D_L)_{5/2} - \frac{h}{2} \right] \\ \dots & \dots \\ -k \left[(D_L)_{n-3/2} + \frac{h}{2} \right] & k \left[(D_L)_{n-3/2} + (D_L)_{n-1/2} \right] * \\ * \left[k (D_L)_{n-1/2} - \frac{h}{2} \right] & -k (D_L)_{n-1/2} & k (D_L)_{n-1/2} \end{bmatrix} \quad (III.38)$$

$$\text{and } \underline{s}'(\theta) = \frac{1}{h^2} \begin{bmatrix} k(D_L)_{1/2} + \frac{h}{2} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (\text{III.39})$$

where $k = \frac{1}{uL}$ and \underline{A}^* , \underline{s} have their usual meaning.

The solution of the matrix differential equation (III.27) is given by *.

$$\underline{w}(\theta) = \underline{D} \underline{Q} \underline{E}(\theta) \underline{Q}^T \underline{D}^{-1} \left[\underline{w}^{(0)}(\theta) + \int_0^\theta \underline{D} \underline{Q} \underline{E}^{-1}(\eta) \underline{Q}^T \underline{D}^{-1} \underline{s}(\eta) d\eta \right] \quad (\text{III.40})$$

where η is a dummy variable

\underline{Q} = The matrix of eigenvectors of \underline{A}

\underline{A} = Original coefficient matrix converted into symmetric i.e. $\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D}$

(As discussed in Chapter II).

\underline{A}^* = Original coefficient matrix

\underline{D} = The diagonal matrix having diagonal elements alternate in sign i.e. $d_i = (-1)^i |d_i|$

$$\underline{E}(\theta) = \begin{bmatrix} e^{-p_1 \theta} & & & \\ & e^{-p_2 \theta} & & \\ & & \ddots & \\ & & & e^{-p_n \theta} \end{bmatrix}; \underline{E}^{-1}(\theta) = \begin{bmatrix} e^{p_1 \theta} & & & \\ & e^{p_2 \theta} & & \\ & & \ddots & \\ & & & e^{p_n \theta} \end{bmatrix} \quad (\text{III.41})$$

* For details of the solution (III.40) refer to Chapter II.

where p_i ($i = 1$ to n) are the n eigenvalues of matrix \underline{A}
 $*$ (as well as \underline{A}^*).

$$\underline{D}^{-1} = \begin{bmatrix} -d_1 & & & \\ & d_2 & & \\ & . & & \\ & . & & \\ & . & & \\ & & & (-1)^n d_n \end{bmatrix} ; \quad \underline{D}^{-1} = \begin{bmatrix} -1/d_1 & & & \\ & 1/d_2 & & \\ & . & & \\ & . & & \\ & . & & \\ & & & (-1)^n 1/d_n \end{bmatrix} \quad (\text{III.42})$$

The results are presented corresponding to the following values of parameters:

$$\left. \begin{aligned} k &= \frac{1}{uL} = 0.3 \\ D_L &= 0.5 (1.0 + z) \\ h &= 0.09524 \\ \underline{w}^{(0)}(\theta) &= 1.0 \quad (\text{Initial condition}) \end{aligned} \right] \quad (\text{III.43})$$

* For proof refer to Appendix A theorem 1.

TABLE III.3

One Dimensional Non-Homogeneous Case:

(Using Ordinary Boundary Conditions).

Summary of Results*; - Ten point grid comparison.

(The results of the ten point grid are derived from those of a twenty point grid using interpolation and compared with the generated values using semi-analytical solution technique).

Grid Point Reduced Time θ	1	3	5	7	9
0.2	0.86238 0.86399 0.00161	0.50770 0.50925 0.00155	0.22353 0.21925 -0.00418	0.07717 0.07126 -0.00591	0.02286 0.01883 -0.00403
0.4	0.94013 0.93972 -0.00041	0.75339 0.75334 -0.00005	0.52763 0.52625 -0.00138	0.32820 0.32446 -0.00374	0.19858 0.19301 -0.00557
0.6	0.96735 0.96624 -0.00111	0.85830 0.85602 -0.00228	0.70687 0.70298 -0.00389	0.54822 0.54288 -0.00534	0.42869 0.42210 -0.00659
0.8	0.98044 0.97898 -0.00146	0.91310 0.90934 -0.00376	0.81444 0.80791 -0.00653	0.70428 0.69563 -0.00865	0.61738 0.60713 -0.01025
1.0	0.98781 0.98615 -0.00166	0.94528 0.94052 -0.00476	0.88196 0.87325 -0.00871	0.80953 0.79759 -0.01194	0.75174 0.73705 -0.01469

*The first entry in each block refers to the value of c , calculated using semi-analytical solution; the second entry refers to the interpolated value; the third entry represents the deviation. interpolated value - the value calculated using semi-analytical technique.

A complete set of results in the tabular form is available in Appendix D.

TABLE III.4

One Dimensional Non-Homogeneous Case.

(Using Danckwerts Boundary Conditions).

Summary of Results*: Ten-point grid comparison.

(The results of the ten point grid are derived from those of a twenty point grid using interpolation and compared with the generated values using semi-analytical solution technique).

Grid Point Reduced Time	1	3	5	7	9
0.2	0.60432 0.60111 -0.00321	0.31488 0.30430 -0.01058	0.12667 0.11565 -0.01102	0.04093 0.03399 -0.00694	0.01152 0.00827 -0.00325
0.4	0.77537 0.77947 0.00410	0.57176 0.57074 -0.00102	0.37128 0.36543 -0.00585	0.21611 0.20782 -0.00829	0.12334 0.11470 -0.00864
0.6	0.85953 0.86376 0.00423	0.72023 0.72139 0.00116	0.55970 0.55673 -0.00297	0.41036 0.40380 -0.00656	0.30545 0.29660 -0.00885
0.8	0.90767 0.91048 0.00281	0.81166 0.81226 0.0006	0.69250 0.68945 -0.00305	6.57249 0.56603 -0.00646	0.48305 0.47393 -0.00912
1.0	0.93760 0.93881 0.00121	0.87105 0.87010 -0.00095	0.78557 0.78100 -0.00457	0.69626 0.68828 -0.00798	0.62819 0.61727 -0.01093

* The first entry in each block refers to the value of c , calculated using semi-analytical technique; the second entry refers to the interpolated value; the third entry represents the deviation: interpolated value - the value generated by semi-analytical solution.

A complete set of results is available in Appendix D.

The matrices \underline{A}^* , \underline{D} , \underline{A} , eigenvalues p_i ($i=1$ to n), and the matrix of eigenvectors are given in appendix D.

The results of a twenty point grid are also presented in Appendix D. Analytical solution to the problem is not available, therefore the values of ten point grid are derived from those of twenty point grid using interpolation. The interpolated values are compared with those of the generated values and the summarized results are shown in tables (III.3) and (III.4).

The complete set of results and the computer programs are given in Appendix D.

2. TWO DIMENSIONAL CASE:

(a) D_R and u Both Functions of R :

This case takes into account the radial variation of the media properties. The fluid is assumed to be axially homogeneous and the velocity profile and the radial dispersion coefficient are taken as dependent upon radial positions. The velocity profile data of Schwartz and Smith (27) and the variation of Peclet number with radial position (accounts for radial variation of diffusivity or the radial dispersion coefficient) as given in (12) are used to account for the radial variation of the properties.

The partial differential equation describing the process is:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u(r) \frac{\partial c}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (r D_R \frac{\partial c}{\partial r}) \quad (\text{III.44})$$

where u and D_R are both functions of r .

To convert equation (III.44) into the dimensionless form, define the following dimensionless groups:

$$Z = \frac{x}{L} \text{ (Dimensionless length, i.e. axial variable).}$$

where L = The characteristic length.

$$R = \frac{r}{R_0} \text{ (Dimensionless radial variable)}$$

where R_0 = The radius of the reactor.

$$\alpha = \frac{D_L}{uL} \text{ (Axial dispersion group)}$$

$$\begin{aligned}
 \beta(R) &= \frac{D_R(R)}{\underline{u} R_O} \quad (\text{Radial dispersion group}) \\
 \theta &= \frac{ut}{L} \quad (\text{Reduced time}) \\
 \gamma &= \frac{L}{R_O} \quad (\text{Constant}) \\
 \eta(R) &= \frac{u(R)}{\underline{u}} = \frac{\text{Point Velocity}}{\text{Average Velocity}}
 \end{aligned}
 \tag{III.45}$$

Substitution of the various dimensionless groups in equation (III.44) after rearranging gives:

$$\frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \eta(R) \frac{\partial C}{\partial z} + \frac{\gamma}{R} \frac{\partial}{\partial R} (R\beta(R) \frac{\partial C}{\partial R})
 \tag{III.46}$$

Equation (III.46) is not applicable at the centre of the reactor. A special equation can be derived to account for this by expanding the last term of equation (III.46)

$$\frac{\gamma}{R} \frac{\partial}{\partial R} (R\beta(R) \frac{\partial C}{\partial R}) = \gamma \beta(R) \frac{\partial^2 C}{\partial R^2} + \gamma \left(\frac{\partial \beta(R)}{\partial R} \right) \frac{\partial C}{\partial R} + \frac{\gamma}{R} \beta(R) \frac{\partial C}{\partial R}
 \tag{III.47}$$

$\therefore \beta(R)$ is constant at the centre

$$\therefore \frac{\partial \beta(R)}{\partial R} = 0
 \tag{III.48}$$

$\therefore \frac{\gamma}{R} \beta(R) \frac{\partial C}{\partial R}$ is intermediate at the centre.

Differentiating the numerator and the denominator of the last term in equation (III.47) w.r.t. R gives:

$$\gamma \frac{\frac{\partial}{\partial R} (\beta(R) \frac{\partial C}{\partial R})}{\frac{\partial}{\partial R} (R)} = \gamma \left(\frac{\partial \beta(R)}{\partial R} \right) \frac{\partial C}{\partial R} + \gamma \beta(R) \frac{\partial^2 C}{\partial R^2}
 \tag{III.49}$$

Substitution of (III.48) in (III.49) gives:

$$\gamma \frac{\frac{\partial}{\partial R} (\beta(R) \frac{\partial C}{\partial R})}{\frac{\partial}{\partial R} (R)} = \gamma \beta(R) \frac{\partial^2 C}{\partial R^2} \quad (\text{III.50})$$

Substituting (III.50) and (III.48) in (III.47) gives:

$$\frac{\gamma}{R} \frac{\partial}{\partial R} (R \beta(R) \frac{\partial C}{\partial R}) = 2 \gamma \beta(R) \frac{\partial^2 C}{\partial R^2} \quad (\text{III.51})$$

Substitution of equation (III.51) in (III.46) gives the equation applicable at the centre:

$$\frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \eta(R) \frac{\partial C}{\partial z} + 2 \gamma \beta(R) \frac{\partial^2 C}{\partial R^2} \quad (\text{III.52})$$

The equation (III.46) along with (III.52) is solved to evaluate the concentration profiles, by discretizing the space derivatives using the following set of finite difference formulations:

$$\left. \begin{aligned} \left(\frac{\partial^2 C}{\partial z^2} \right)_{i,j} &= \frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{h^2} \\ \left(\frac{\partial C}{\partial z} \right)_{i,j} &= \frac{C_{i+1,j} - C_{i-1,j}}{2h} \\ \left(\frac{\partial^2 C}{\partial R^2} \right)_{i,j} &= \frac{C_{i,j+1} - 2C_{i,j} + C_{i,j-1}}{k^2} \\ \left[\frac{1}{R} \frac{\partial}{\partial R} (R \beta(R) \frac{\partial C}{\partial R}) \right]_{i,j} &= \frac{1}{(R)_{i,j}} \left[\left[R \beta(R) \right]_{i,j+1/2} (C_{i,j+1} - C_{i,j}) \right. \\ &\quad \left. - \left[R \beta(R) \right]_{i,j-1/2} (C_{i,j} - C_{i,j-1}) / k^2 \right] \end{aligned} \right\} \quad (\text{III.53})$$

where h = The grid spacing in the axial direction.

and k = The grid spacing in the radial direction.

The variation of radial dispersion coefficient and hence radial dispersion group in the radial direction is derived from the peclet number variation as suggested by Fahein and Smith (12):

$$Pe = Pe_o + F(R)^m \quad (III.54)$$

where Pe = The point peclet number

Pe_o = The value of peclet number at the centre which is taken as 8.

R = The radial position.

m, F = Constants depending upon particle diameter and tube diameter.

Various sets of equations can be derived using (III.54) depending upon particle dia. and tube dia. The relationships, in the form of graphs, of F and m in terms of the ratio d_p/d_T (Particle dia/Tube dia) are available in (12).

A particular set has been derived using the following values:

Particle diameter = 0.5" spheres

Tube diameter = 8.0"

$$Pe = 8.0 + 15(R)^6 \quad (III.55)$$

$$\therefore Pe = \frac{d_p u}{D_R(R)} \quad (III.56)$$

Multiplying the numerator and denominator of equation (III.56) by d_2 and rearranging:

$$Pe = \left(\frac{d_p}{d_T}\right) \left(\frac{d_T u_{av}}{D_R(R)}\right)$$

or

$$Pe = \left(\frac{d_p}{d_T}\right) / 2\beta(R) \quad (III.56)$$

$$\therefore d_T = 2R_o \text{ where } R_o = \text{Radius of the tube}$$

and $\beta(R) = \frac{D_R(R)}{u_{av} R_o}$ (Radial dispersion group)

Combining equations (III.55) and (III.56) gives after rearranging:

$$\beta(R) = \frac{2(d_p/d_T)}{8.0 + 15(R)^6} \quad (III.57)$$

Hence equation (III.57) represents the variation of the radial dispersion group with the radial position.

The solution to the upper half of the reactor was obtained because of the radial symmetry. The partial differential equation (III.46) along with (III.52) is discretized using the finite difference formulations as given by equation (III.53) to get a set of ordinary differential equations as given below. The grid is as shown in figure III-d.

$$\frac{dc_1}{d\theta} = \frac{1}{h^2} \left[-(2\alpha + 4\gamma\beta(R))c_1 + \left(\alpha - \frac{h}{2}\eta(R)\right)c_2 + 4\gamma\beta(R)c_6 \right] + \frac{1}{h^2} \left(\alpha + \frac{h}{2}\eta(R)\right)$$

(III.58.1)

$$\frac{dc_2}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2} \eta(R) \right) c_1 - (2\alpha + 4\gamma\beta(R)) c_2 + \left(\alpha - \frac{h}{2} \eta(R) \right) c_3 + 4\gamma\beta(R) c_7 \right]$$

(III.58.2)

$$\frac{dc_3}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2} \eta(R) \right) c_2 - (2\alpha + 4\gamma\beta(R)) c_3 + \left(\alpha - \frac{h}{2} \eta(R) \right) c_4 + 4\gamma\beta(R) c_8 \right]$$

(III.58.3)

$$\frac{dc_4}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2} \eta(R) \right) c_3 - (2\alpha + 4\gamma\beta(R)) c_4 + \left(\alpha - \frac{h}{2} \eta(R) \right) c_5 + 4\gamma\beta(R) c_9 \right]$$

(III.58.4)

$$\frac{dc_5}{d\theta} = \frac{1}{h^2} \left[\left(\alpha + \frac{h}{2} \eta(R) \right) c_4 - \left(\alpha + \frac{h}{2} \eta(R) + 4\gamma\beta(R) \right) c_5 + 4\gamma\beta(R) c_{10} \right]$$

(III.58.5)

$$\begin{aligned} \frac{dc_6}{d\theta} = \frac{1}{h^2} & \left[\frac{\gamma}{k} (R\beta(R))_{1,1/2} c_1 - \left[\left(2\alpha + \frac{\gamma}{k} (R\beta(R))_{1,1/2} + (R\beta(R))_{1,1/2} \right) c_6 \right. \right. \\ & \left. \left. + \left(\alpha - \frac{h}{2} \eta(R) \right) c_7 + \frac{\alpha}{k} (R\beta(R))_{1,3/2} c_{11} \right] + \frac{1}{h^2} \left(\alpha + \frac{h}{2} \eta(R) \right) \right] \end{aligned}$$

(III.58.6)

$$\begin{aligned} \frac{dc_7}{d\theta} = \frac{1}{h^2} & \left[\frac{\gamma}{k} (R\beta(R))_{2,1/2} c_2 + \left(\alpha + \frac{h}{2} \eta(R) \right) c_6 - \left[\left(2\alpha + \frac{\gamma}{k} (R\beta(R))_{2,3/2} \right. \right. \right. \\ & \left. \left. + (R\beta(R))_{2,1/2} \right) c_7 + \left(\alpha - \frac{h}{2} \eta(R) \right) c_8 + \frac{\gamma}{k} (R\beta(R))_{2,3/2} c_{12} \right] \end{aligned}$$

(III.58.7)

$$\begin{aligned} \frac{dc_8}{d\theta} = \frac{1}{h^2} & \left[\frac{\gamma}{k} (R\beta(R))_{3,1/2} c_3 + \left(\alpha + \frac{h}{2} \eta(R) \right) c_7 - \left[\left(2\alpha + \frac{\gamma}{k} (R\beta(R))_{3,3/2} \right. \right. \right. \\ & \left. \left. + (R\beta(R))_{3,1/2} \right) c_8 + \left(\alpha - \frac{h}{2} \eta(R) \right) c_9 + \frac{\gamma}{k} (R\beta(R))_{3,3/2} c_{13} \right] \end{aligned}$$

(III.58.8)

$$\frac{dc_9}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{k} (R\beta(R))_{4,1/2} c_4 + \left(\alpha + \frac{h}{2} \eta(R) \right) c_8 - \left[2\alpha + \frac{\gamma}{k} (R\beta(R))_{4,3/2} + (R\beta(R))_{4,1/2} \right] c_9 + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{10} + \frac{\gamma}{k} (R\beta(R))_{4,3/2} c_{14} \right]$$

(III.58.9)

$$\frac{dc_{10}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{k} (R\beta(R))_{5,1/2} c_5 + \left(\alpha + \frac{h}{2} \eta(R) \right) c_9 - \left[\left(\alpha + \frac{h}{2} \eta(R) \right) + \frac{\gamma}{k} (R\beta(R))_{5,1/2} + (R\beta(R))_{5,3/2} \right] c_{10} + \frac{\gamma}{k} (R\beta(R))_{5,3/2} c_{15} \right]$$

(III.58.10)

$$\frac{dc_{11}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{2k} (R\beta(R))_{1,3/2} c_6 - \left[\left(2\alpha + \frac{\gamma}{2k} (R\beta(R))_{1,5/2} + (R\beta(R))_{1,3/2} \right) c_{11} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{12} + \frac{\gamma}{2k} (R\beta(R))_{1,5/2} c_{16} \right] + \frac{1}{h^2} \left(\alpha + \frac{h}{2} \eta(R) \right) \right]$$

(III.58.11)

$$\frac{dc_{12}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{2k} (R\beta(R))_{2,3/2} c_7 + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{11} - \left[\left(2\alpha + \frac{\gamma}{2k} (R\beta(R))_{2,5/2} + (R\beta(R))_{2,3/2} \right) c_{12} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{13} + \frac{\gamma}{2k} (R\beta(R))_{2,5/2} c_{17} \right] \right]$$

(III.58.12)

$$\frac{dc_{13}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{2k} (R\beta(R))_{3,3/2} c_8 + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{12} - \left[\left(2\alpha + \frac{\gamma}{2k} (R\beta(R))_{3,5/2} + (R\beta(R))_{3,3/2} \right) c_{13} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{14} + \frac{\gamma}{2k} (R\beta(R))_{3,5/2} c_{18} \right] \right]$$

(III.58.13)

$$\frac{dc_{14}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{2k} (R\beta(R))_{4,3/2} c_9 + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{13} - \left[2\alpha + \frac{\gamma}{2k} (R\beta(R))_{4,5/2} + \right. \right. \\ \left. \left. (R\beta(R))_{4,3/2} \right] c_{14} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{15} + \frac{\gamma}{2k} (R\beta(R))_{4,5/2} c_{19} \right] \\ \text{(III.58.14)}$$

$$\frac{dc_{15}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{2k} (R\beta(R))_{5,3/2} c_{10} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{14} - \left[\left(\alpha + \frac{h}{2} \eta(R) \right) + \frac{\gamma}{2k} \right. \right. \\ \left. \left. ((R\beta(R))_{5,3/2} (R\beta(R))_{5,3/2}) \right] c_{15} + \frac{\gamma}{2k} (R\beta(R))_{5,5/2} c_{20} \right] \\ \text{(III.58.15)}$$

$$\frac{dc_{16}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{3k} (R\beta(R))_{1,5/2} c_{11} - \left[2\alpha + \frac{\gamma}{3k} ((R\beta(R))_{1,5/2} + (R\beta(R))_{1,7/2}) \right. \right. \\ \left. \left. c_{16} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{17} + \frac{\gamma}{3k} (R\beta(R))_{1,7/2} c_{21} \right] + \frac{1}{h^2} \left(\alpha + \frac{h}{2} \eta(R) \right) \right] \\ \text{(III.58.16)}$$

$$\frac{dc_{17}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{3k} (R\beta(R))_{2,5/2} c_{12} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{16} - \left[2\alpha + \frac{\gamma}{3k} (R\beta(R))_{2,5/2} + \right. \right. \\ \left. \left. (R\beta(R))_{2,7/2} \right] c_{17} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{18} + \frac{\gamma}{3k} (R\beta(R))_{2,7/2} c_{22} \right] \\ \text{(III.58.17)}$$

$$\frac{dc_{18}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{3k} (R\beta(R))_{3,5/2} c_{13} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{17} - \left[2\alpha + \frac{\gamma}{3k} (R\beta(R))_{3,5/2} \right. \right. \\ \left. \left. (R\beta(R))_{3,7/2} \right] c_{18} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{19} + \frac{\gamma}{3k} (R\beta(R))_{3,7/2} c_{23} \right] \quad (\text{III.58.18})$$

$$\frac{dc_{19}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{3k} (R\beta(R))_{4,5/2} c_{14} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{18} - \left[2\alpha + \frac{\gamma}{3k} (R\beta(R))_{4,5/2} \right. \right. \\ \left. \left. + (R\beta(R))_{4,7/2} \right] c_{19} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{20} + \frac{\gamma}{3k} (R\beta(R))_{4,7/2} c_{24} \right] \quad (\text{III.58.19})$$

$$\frac{dc_{20}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{3k} (R\beta(R))_{5,5/2} c_{15} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{19} - \left[\left(\alpha + \frac{h}{2} \eta(R) \right) + \frac{\gamma}{3k} \right. \right. \\ \left. \left. (R\beta(R))_{5,5/2} + (R\beta(R))_{5,7/2} \right] c_{20} + \frac{\gamma}{3k} (R\beta(R))_{5,7/2} c_{25} \right] \quad (\text{III.58.20})$$

$$\frac{dc_{21}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{4k} (R\beta(R))_{1,7/2} c_{16} - \left[2\alpha + \frac{\gamma}{4k} (R\beta(R))_{1,7/2} + (R\beta(R))_{1,9/2} \right] \right. \\ \left. c_{21} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{22} + \frac{\gamma}{4k} (R\beta(R))_{1,9/2} c_{26} \right] + \frac{1}{h^2} \left(\alpha + \frac{h}{2} \eta(R) \right) \quad (\text{III.58.21})$$

$$\frac{dc_{22}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{4k} (R\beta(R))_{2,7/2} c_{17} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{21} - \left[2\alpha + \frac{\gamma}{4k} (R\beta(R))_{2,7/2} \right. \right. \\ \left. \left. + (R\beta(R))_{2,9/2} \right] c_{22} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{23} + \frac{\gamma}{4k} (R\beta(R))_{2,9/2} c_{27} \right] \quad (\text{III.58.22})$$

$$\frac{dc_{23}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{4k} (R\beta(R))_{3,7/2} c_{18} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{22} - \left[2\alpha + \frac{\gamma}{4k} (R\beta(R))_{3,7/2} \right. \right. \\ \left. \left. + (R\beta(R))_{3,9/2} \right] c_{23} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{24} + \frac{\gamma}{4k} (R\beta(R))_{3,9/2} c_{28} \right] \quad (\text{III.58.23})$$

$$\frac{dc_{24}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{4k} (R\beta(R))_{4,7/2} c_{19} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{23} - \left[2\alpha + \frac{\gamma}{4k} (R\beta(R))_{4,7/2} \right. \right. \\ \left. \left. + (R\beta(R))_{4,9/2} \right] c_{24} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{25} + \frac{\gamma}{4k} (R\beta(R))_{4,9/2} c_{28} \right] \quad (\text{III.58.24})$$

$$\frac{dc_{25}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{4k} (R\beta(R))_{5,7/2} c_{20} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{24} - \left[\left(\alpha + \frac{h}{2} \eta(R) \right) + \frac{\gamma}{4k} (R\beta(R))_{5,7/2} \right. \right. \\ \left. \left. + (R\beta(R))_{5,9/2} \right] c_{25} + \frac{\gamma}{4k} (R\beta(R))_{5,9/2} c_{30} \right] \quad (\text{III.58.25})$$

$$\frac{dc_{26}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{5k} (R\beta(R))_{1,9/2} c_{21} - \left[2\alpha + \frac{\gamma}{5k} (R\beta(R))_{1,9/2} \right] c_{26} \right. \\ \left. + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{27} + \frac{1}{h} \left(\alpha + \frac{h}{2} \eta(R) \right) \right] \quad (\text{III.58.26})$$

$$\frac{dc_{27}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{5k} (R\beta(R))_{2,9/2} c_{22} + \left(\alpha + \frac{h}{2} \eta(R) \right) c_{26} - \left[2\alpha + \frac{\gamma}{5k} (R\beta(R))_{2,9/2} \right] \right. \\ \left. c_{27} + \left(\alpha - \frac{h}{2} \eta(R) \right) c_{28} \right] \quad (\text{III.58.27})$$

$$\frac{dc_{28}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{5k} (R\beta(R))_{3,9/2} c_{23} + \left(\alpha + \frac{h}{2}\eta(R)\right) c_{27} - \left[2\alpha + \frac{\gamma}{5k} (R\beta(R))_{3,9/2} \right] c_{28} + \left(\alpha - \frac{h}{2}\eta(R)\right) c_{29} \right] \quad (\text{III.58.28})$$

$$\frac{dc_{29}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{5k} (R\beta(R))_{4,9/2} + \left(\alpha + \frac{h}{2}\eta(R)\right) c_{28} - \left[2\alpha + \frac{\gamma}{5k} (R\beta(R))_{4,9/2} \right] c_{29} + \left(\alpha - \frac{h}{2}\eta(R)\right) c_{30} \right] \quad (\text{III.58.29})$$

$$\frac{dc_{30}}{d\theta} = \frac{1}{h^2} \left[\frac{\gamma}{5k} (R\beta(R))_{5,9/2} c_{25} + \left(\alpha + \frac{h}{2}\eta(R)\right) c_{29} - \left[\left(\alpha + \frac{h}{2}\eta(R)\right) + \frac{\gamma}{5k} (R\beta(R))_{5,9/2} \right] c_{30} \right] \quad (\text{III.58.30})$$

The set of ordinary differential equations (III.58.1) through (III.58.30) can be represented by the following matrix differential equation as discussed earlier:

$$\frac{d\underline{w}(\theta)}{d\theta} = - \underline{A}^* \underline{w}(\theta) + \underline{s}'(\theta) \quad (\text{III.59})$$

where \underline{A}^* = The original coefficient matrix.

$\underline{s}'(\theta)$ = The boundary condition vector.

$\underline{w}(\theta)$ = The vector of unknowns.

This case was tried but the eigenvalues of the original coefficient matrix did not converge even after 90 iterations corresponding an error criteria of 0.001.

* $\underline{c}(\theta)$ and $\underline{w}(\theta)$ have the same meaning here.

(b) Only D_R a function of R .

This case is simpler as compared to the one discussed earlier. The velocity profile is assumed to be flat and the variation of radial dispersion group with radial position is as given by (III.57) corresponding to a particular set of variables as defined there.

The partial differential equation describing this process is:

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - u \frac{\partial C}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (r D_R \frac{\partial C}{\partial r}) \quad (\text{III.60})$$

Define the dimensionless quantities as given by (III.45) except $\eta(R)$ which is now unity. On rearranging and substituting the values we get:

$$\frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} + \frac{\gamma}{R} \frac{\partial}{\partial R} (R \beta(R) \frac{\partial C}{\partial R}) \quad (\text{III.61})$$

The partial differential equation applicable at the centre is given by:

$$\frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} + 2\gamma \beta(R) \frac{\partial^2 C}{\partial z^2} \quad (\text{III.62})$$

Taking advantage of the radial symmetry, the solution to the upper half of the reactor is obtained. The finite difference grid is as shown in figure III-d.

Both the partial differential equations (III.61) and (III.62) are discretized using the set of finite difference formulations as given by (III.53) to get a set of ordinary differential equations. This set is a particular case of the previous set defined by (III.58.1) through (III.58.30) and can be derived by substituting $n(R) = 1$ in that set.

The set of ordinary differential equations can be represented by a single matrix differential equation (III.59). The matrix \underline{A}^* is converted into the real symmetric matrix \underline{A} using similarity transformation $\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D}$ as discussed in Chapter II. For the details of various matrices and the corresponding results, the reference is made to the Appendix C1. The results of this model are compared with the simpler one dimensional model and the details are given in Chapter V.

C. EIGENVALUES AND EIGENVECTORS OF A

The original coefficient matrix \underline{A}^* as discussed earlier is converted to the real symmetric form using similarity transformation. The methods used for finding out the eigenvalues and eigenvectors of a symmetric matrix can be classified in two main categories:

1. Non-Iterative or Direct Methods: These methods are more time-consuming on the computer and involve a large number of multiplications. The methods belonging to this

category are those due to Leverrier, Hessenberg, and Givens. Some details of these methods are described in Lapidus (18).

2. Iterative Methods: These methods are mostly used on the digital computer. These methods are advantageous in certain respects as compared to the direct methods, namely;

- (a) All the eigenvalues are determined at the same time.
- (b) Using a set of orthogonal transformations, all the eigenvectors are determined simultaneously.

Some of these methods are those due to Jacobi (25) and Householder (33).

Complete details of these methods are available in various books on numerical analysis and the development of the algorithms is not attempted here. Jacobi's method has been used in this thesis and a brief descriptions of the method is presented here.

Jacobi's Method: This method applies to real, symmetric and Hermetian matrices and it yields all the roots at one time. The procedure involves the annihilation of the off diagonal elements using a series of orthogonal matrices. The procedure is illustrated considering a second order matrix A. A new matrix B is formed by the transformation:

$$\underline{B} = \underline{Q}_1^T \underline{A} \underline{Q}_1 \quad (\text{III.63})$$

where

$$\underline{Q_1} = \begin{bmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{bmatrix} \quad (\text{III.64})$$

The transformation of this type is known as Rotation.

Now if the off diagonal elements of matrix B are to be zero, then the following equation or identity must be satisfied.

$$\tan 2\alpha = \frac{2a_{12}}{a_{11} - a_{22}} \quad (\text{III.65})$$

and the choice of α as given in (III.65) annihilates the off diagonal elements. The main diagonal elements of B are p_1 and p_2 , the eigenvalues of A (the eigenvalues of A and B are same since they are similar).

In the case A of order n , the Q₁ matrix is replaced by:

$$\underline{Q_1} = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & (\cos \alpha)_{ii} \dots \dots \dots (-\sin \alpha)_{ij} & & \\ & & & \dots \dots \dots 1 \dots \dots \dots & & \\ & & & & (\sin \alpha)_{ji} \dots \dots \dots (\cos \alpha)_{jj} & \\ & & & & & 1 \\ & & & & & & 1 \end{bmatrix} \quad (\text{III.66})$$

This is modified identity matrix with $\cos \alpha$ as the i^{th} and j^{th} diagonal elements, $\sin \alpha$ as the j^{th} row and i^{th} column element and $-\sin \alpha$ as the i^{th} row and j^{th} column element. This will annihilate the element a_{ij} and a_{ji} . The value of α is given by the following expression:

$$\tan 2\alpha = \frac{2a_{ij}}{a_{ii} - a_{jj}} \quad (\text{III.67})$$

The largest off diagonal elements is first annihilated, but it can take a non-zero value at a later stage. Hence the method has no fixed number of iterations.

The result is given by the following equation when the required convergence has been achieved.

$$\underline{Q}_r^T \underline{Q}_{r-1}^T \dots \underline{Q}_2^T \underline{Q}_1^T \underline{A} \underline{Q}_1 \underline{Q}_2 \dots \underline{Q}_{r-1} \underline{Q}_r = \underline{P} \quad (\text{III.68})$$

where r refers to the number of iterations and \underline{P} is the diagonal matrix of eigenvalues of \underline{A} .

If the matrix $\underline{Q}_1 \underline{Q}_2 \dots \underline{Q}_{r-1} \underline{Q}_r$ is denoted by \underline{Q} and $\underline{Q}_r^T \underline{Q}_{r-1}^T \dots \underline{Q}_2^T \underline{Q}_1^T$ by \underline{Q}^T , the overall transformation is given by

$$\underline{Q}^T \underline{A} \underline{Q} = \underline{P} \quad (\text{III.69})$$

Premultiplication by \underline{Q} gives:

$$\underline{A} \underline{Q} = \underline{Q} \underline{P} \quad (\text{III.70})$$

where \underline{Q} = The matrix of eigenvectors of \underline{A} .

IV. FORWARD PROBLEM

(HIGHER ORDER CORRECT MONOTONE TYPE FINITE DIFFERENCE FORMULATIONS)

In this chapter the solutions to the dispersion model equation, one dimensional homogeneous case, is presented using higher order correct monotone type formulations as suggested by Bramble and Hubbard (6) and Price (22). The computational molecules used in deriving the coefficient matrices are presented in figure IV-a.

No analytical solution is available corresponding to the various sets of boundary conditions used in this thesis. Therefore to get an overall idea of the accuracy of the problem the results of a lower point grid are derived from those of a higher point grid and compared. The accuracy of the various finite difference formulations is tested using the analytical solution to the problem (4) for some other boundary conditions. The coefficient matrices are developed for each of these cases and the techniques used for finding out the eigenvalues and the eigenvectors of the coefficient matrix are also discussed in some detail at the end of this chapter.

Two types of finite difference formulations have been used depending upon the significance of the convective term as discussed in chapter II.

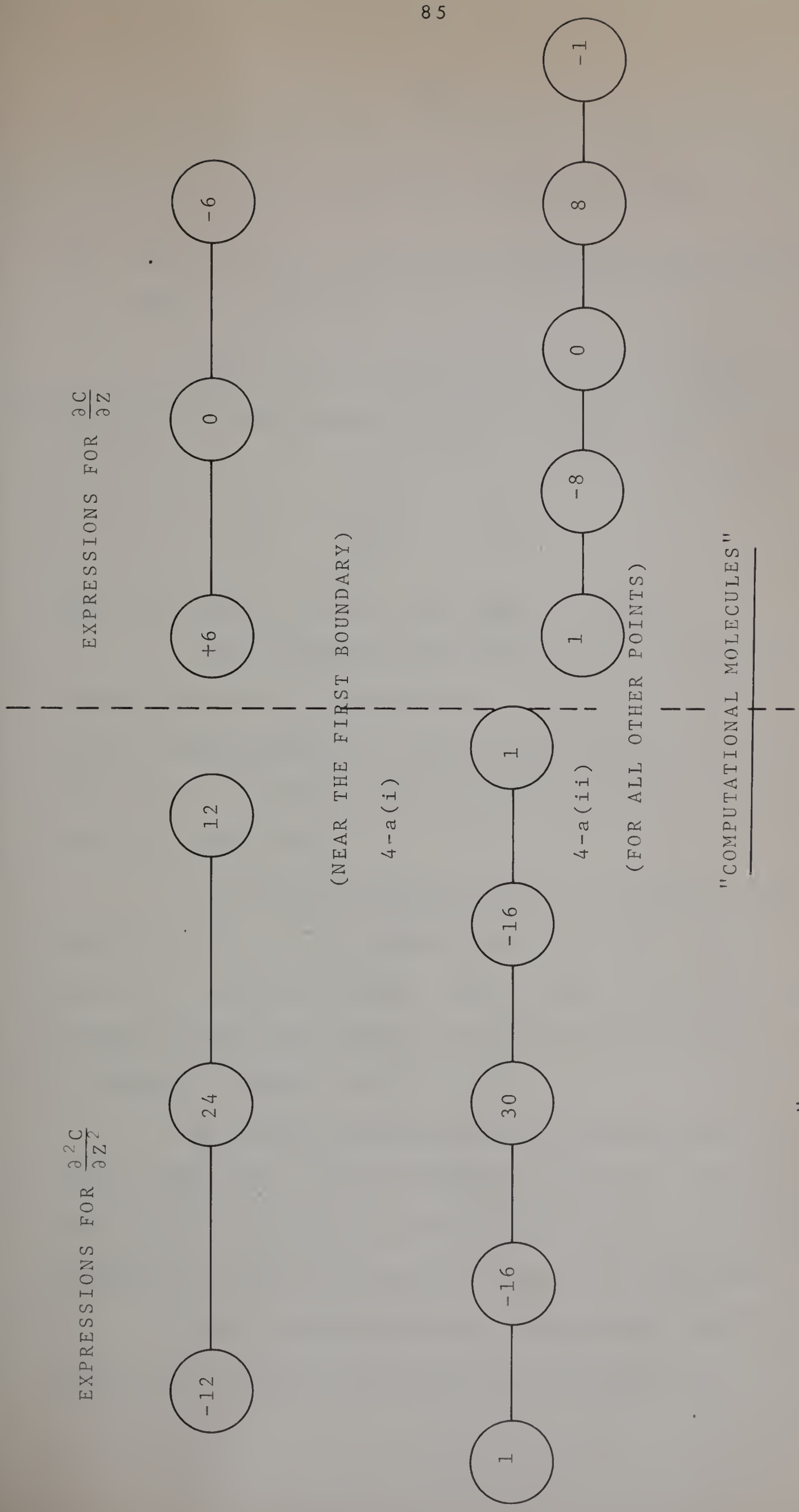


FIGURE IV-a

HIGHER ORDER CORRECT MONOTONE TYPE FINITE DIFFERENCE APPROXIMATIONS

A. ONE DIMENSIONAL HOMOGENEOUS CASE

(a) USING CENTRAL DIFFERENCE SCHEME FOR THE CONVECTIVE
TERM $(\partial c / \partial z) :-$

The partial differential equation describing one dimensional homogeneous problem is given by:

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} \quad (\text{IV.1})$$

where the symbols have their usual meaning.

The concentration profiles are studied using the finite difference formulations as given by (IV.2) and (IV.3) corresponding to a particular value of α . The equation (IV.1) is solved using ordinary as well as Danckwerts boundary conditions.

A finite difference grid is considered and the length $(0 \leq z \leq 1)$ is divided into a finite number of increments (n) of width h each, with a slab of width $\frac{h}{2}$ near the boundary where the value of the flux is specified. The grid is shown in figure IV-b.

By discretizing the space derivatives of equation (IV.2) using the finite difference sets as given by (IV.2) and (IV.3), the partial differential equation can be transformed to a set of ordinary differential equations.

The finite difference expressions used in deriving the set of ordinary differential equations are:

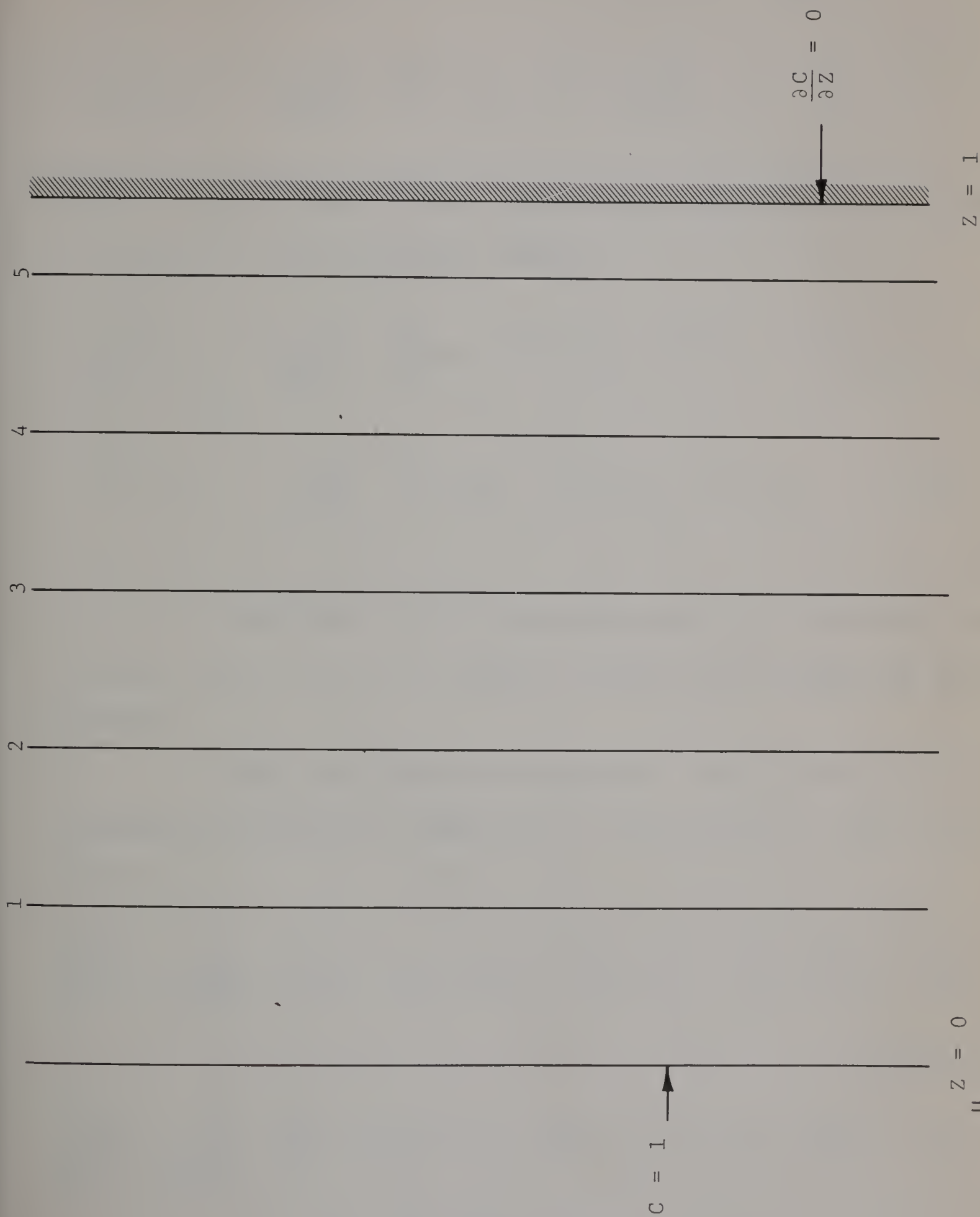


FIGURE IV-b
ILLUSTRATION OF A FIVE POINT GRID ONE DIMENSIONAL HOMOGENEOUS CASE

$$\left(\frac{\partial^2 c}{\partial z^2} \right)_i = \frac{1}{12h^2} \left[-12 c_{i-1} + 24 c_i - 12 c_{i+1} \right]$$

$$\left(\frac{\partial c}{\partial z} \right)_i = \frac{1}{12h^2} \left[6h c_{i-1} - 6h c_{i+1} \right] \quad (\text{IV.2})$$

The above set is applicable for only $i = 1$, where i refers to the grid point number.

$$\left(\frac{\partial^2 c}{\partial z^2} \right)_i = -\frac{1}{12h^2} \left[c_{i+2} - 16 c_{i+1} + 30 c_i - 16 c_{i-1} + c_{i-2} \right]$$

$$\left(\frac{\partial c}{\partial z} \right)_i = -\frac{1}{12h^2} \left[h c_{i+2} - 8h c_{i+1} + 8h c_{i-1} - h c_{i-2} \right] \quad (\text{IV.3})$$

The above set is applicable for all the other grid points i.e. $i = 2$ to n (where n is the total number of grid points).

Using the above expressions, the following set of ordinary differential equations is derived for a five point grid:

$$\frac{dc_1}{d\theta} = \frac{1}{12h^2} \left[-24\alpha c_1 + 12 \left(\alpha - \frac{h}{2} \right) c_2 \right] + \frac{1}{12h^2} \left[12 \left(\alpha + \frac{h}{2} \right) \right]$$

(IV.4.1)

$$\frac{dc_2}{d\theta} = \frac{1}{12h^2} \left[16 \left(\alpha + \frac{h}{2} \right) c_1 - 30\alpha c_2 + 16 \left(\alpha - \frac{h}{2} \right) c_3 - (\alpha - h) c_4 \right]$$

$$- \frac{1}{12h^2} \left[\alpha + h \right] \quad (\text{IV.4.2})$$

$$\frac{dc_3}{d\theta} = \frac{1}{12h^2} \left[-(\alpha + h) c_1 + 16 \left(\alpha + \frac{h}{2}\right) c_2 - 30\alpha c_3 + 16 \left(\alpha - \frac{h}{2}\right) c_4 - (\alpha - h) c_5 \right] \quad (\text{IV.4.3})$$

$$\frac{dc_4}{d\theta} = \frac{1}{12h^2} \left[-(\alpha + h) c_2 + 16 \left(\alpha + \frac{h}{2}\right) c_3 - 30\alpha c_4 + (15\alpha - 7h) c_5 \right] \quad (\text{IV.4.4})$$

$$\frac{dc_5}{d\theta} = \frac{1}{12h^2} \left[-(\alpha + h) c_3 + (15\alpha + 9h) c_4 - (14\alpha - 8h) c_5 \right] \quad (\text{IV.4.5})$$

To satisfy the second boundary condition the following equations are employed:

$$c_{i+2} = c_{i+1} \quad (\text{for } i = 4) \quad (\text{IV.4.6})$$

$$\left. \begin{aligned} c_{i+1} &= c_i \\ c_{i+2} &= c_{i-1} \end{aligned} \right\} \quad (\text{for } i = 5) \quad (\text{IV.4.7})$$

The set of ordinary differential equations (IV.4.1) through (IV.4.5) may be put in the form of the following matrix differential equation:

$$\frac{d}{d\theta} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} = - \frac{1}{12h^2} \begin{bmatrix} 24\alpha & -12(\alpha - \frac{h}{2}) & & & \\ -16(\alpha + \frac{h}{2}) & 30\alpha & -16(\alpha - \frac{h}{2}) & (\alpha - h) & \\ (\alpha + h) & -16(\alpha + \frac{h}{2}) & 30\alpha & -16(\alpha - \frac{h}{2}) & (\alpha - h) \\ & (\alpha + h) & -16(\alpha + \frac{h}{2}) & 30\alpha & -(15\alpha - 7h) \\ & & (\alpha + h) & -(15\alpha + 9h) & (14\alpha + 8h) \end{bmatrix}$$

$$x \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} + \frac{1}{12h^2} \begin{bmatrix} 12(\alpha + \frac{h}{2}) \\ -(\alpha + h) \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (IV.5)$$

According to equation (III.31) the various matrices can be designated as:

$$\underline{A}^* = \frac{1}{12h^2} \begin{bmatrix} 24\alpha & -12(\alpha - \frac{h}{2}) & & & \\ -16(\alpha + \frac{h}{2}) & 30\alpha & -16(\alpha - \frac{h}{2}) & (\alpha - h) & \\ (\alpha + h) & -16(\alpha + \frac{h}{2}) & 30\alpha & -16(\alpha - \frac{h}{2}) & (\alpha - h) \\ & (\alpha + h) & -16(\alpha + \frac{h}{2}) & 30\alpha & -(15\alpha - 7h) \\ & & (\alpha + h) & -(15\alpha + 9h) & (14\alpha + 8h) \end{bmatrix}$$

and

$$\underline{s}'(\theta) = \frac{1}{12h^2} \begin{bmatrix} 12(\alpha + \frac{h}{2}) \\ -(\alpha + h) \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (IV.6)$$

The coefficient matrix \underline{A}^* in this case is unsymmetric and it satisfies the following conditions as given in (22) i.e.

The matrix \underline{A}^* is monotone and there exists a real (nxn) matrix \underline{R} which satisfies the following properties:

$$\underline{M} = \underline{A}^* + \underline{R} \text{ is monotone}$$

$$\underline{M}^{-1} \underline{R} \geq 0 \quad (\text{IV.7})$$

$$\rho(\underline{M}^{-1} \underline{R}) < 1$$

where ρ is the spectral radius of $(\underline{M}^{-1} \underline{R})$, and is defined by:

$$\rho(\underline{M}^{-1} \underline{R}) \equiv \text{Max } |\lambda_i| \quad (\text{IV.8})$$

where λ_i , ($i = 1$ to n) are the eigenvalues of (nxn) matrix $(\underline{M}^{-1} \underline{R})$.

The solution of the matrix differential equation (IV.5) is given by:

$$\underline{c}(\theta) = \underline{Q} \underline{E}(\theta) \underline{Q}^{-1} \left[\underline{c}^{(0)}(\theta) + \int_0^\theta \underline{Q} \underline{E}^{-1}(\eta) \underline{Q}^{-1} \underline{s}(\eta) d\eta \right] \quad (\text{IV.9})$$

where η is a dummy variable

$$\underline{c}^{(0)}(\theta) = \text{Initial condition vector}$$

$$\underline{Q} = \text{The matrix of eigenvectors of } \underline{A}^*$$

$$\begin{aligned}\underline{Q}^{-1} &= \text{Inverse of the matrix of eigenvectors} \\ \underline{s}(\eta) &= \text{The boundary condition vector}\end{aligned}$$

The equation (IV.5) is solved using both sets of boundary conditions as described previously. The matrix satisfying the properties given by (IV.7) has got all its eigenvalues real, positive and distinct.

The following parameters are used

$$\left. \begin{aligned}\alpha &= 0.2 \\ h &= 0.1818 \\ n &= 5 \\ \underline{c}^{(0)}(\theta) &= \underline{0}\end{aligned}\right\} \quad (\text{IV.10})$$

and the results are presented in Appendix E. The coefficient matrix \underline{A}^* , eigenvalues, and the matrix eigenvectors \underline{Q} are also given in Appendix E.

The results of a five point grid are derived from those of a ten point grid and compared with the values using semi-analytical solution, in order to get an overall idea of the accuracy. A summary of results corresponding to both sets of boundary conditions is presented in the tabular form in the tables IV.1 and IV.2.

The relevant computer programs along with the complete set of results are given in Appendix E.

TABLE IV.1

One Dimensional Homogeneous Case
(Using Ordinary Boundary Conditions)

Higher Order Correct Monotone Type Finite Difference Formulations.

Summary of Results* Five point Grid Comparison. (The results of a five point grid are derived from those of a ten point grid using interpolation and compared with the generated values using semi-analytical solution)

Reduced Time θ \ Grid Point	1	3	5
0.2	0.72989 0.74330 0.01341	0.18264 0.17610 -0.00654	0.01355 0.01092 -0.00263
0.4	0.88411 0.88846 0.00435	0.49256 0.49707 0.00451	0.17797 0.17518 -0.00279
0.6	0.94010 0.94133 0.00123	0.69250 0.69674 0.00424	0.41678 0.42057 0.00347
0.8	0.96611 0.96661 0.00050	0.81227 0.81550 0.00323	0.61678 0.62266 0.00588
1.0	0.97993 0.98041 0.00048	0.88469 0.88758 0.00289	0.75655 0.76227 0.00572

*The first entry in each block refers to the value of C, calculated by semi-analytical solutions; the second entry refers to the interpolated value; the third entry represents the deviation:- interpolated value - the value generated using semi-analytical technique.

A complete set of results is available in Appendix E.

TABLE IV.2

One Dimensional Homogeneous Case
(Using Danckwerts Boundary Conditions)

Higher Order Correct Monotone Type Finite Difference Formulations.

Summary of Results*. Five point Grid Comparison (The results of a five point grid are derived from those of a ten point grid using interpolation and compared with the generated values using the semi-analytical solution technique).

Grid Point Reduced Time θ	1	3	5
0.2	0.48194 0.46871 -0.01323	0.10524 0.08879 -0.01645	0.00705 0.00468 -0.00237
0.4	0.68654 0.68892 0.00238	0.33571 0.32574 -0.00997	0.10957 0.09878 -0.01079
0.6	0.79872 0.80491 0.00619	0.52845 0.52654 -0.00191	0.28894 0.28114 -0.00780
0.8	0.86657 0.87323 0.00666	0.66954 0.67242 0.00288	0.46854 0.46695 0.00159
1.0	0.90989 0.91606 0.00617	0.76962 0.77503 0.00541	0.61630 0.61958 0.00328

* The first entry in each block refers to the value of C, calculated by semi-analytical solution; the second entry refers to the interpolated value; the third entry represents the deviation:- interpolated value - the value generated using semi-analytical solution.

A complete set of results is available in Appendix E.

B. USING BACKWARD DIFFERENCE SCHEME (24) FOR THE CONVECTIVE

$$\text{TERM } \left(\frac{\partial c}{\partial z} \right) :-$$

In many problems the convective term is large and for such cases Price et al (24) suggests the second order correct backward difference approximation for the convective term as given by (II.10) and is

$$\frac{\partial c}{\partial z} = \frac{0.5 c_{i-2} - 2 c_{i-1} + 1.5 c_i}{h} \quad (\text{IV.11})$$

The above equation may be used for all grid points except for those next to the boundary where one has to be satisfied with first order correct expressions.

The equation (IV.1) can be discretized using the finite difference formulations (IV.12) and (IV.13).

$$\left(\frac{\partial^2 c}{\partial z^2} \right)_i = - \frac{1}{12h^2} \left[-12 c_{i-1} + 24 c_i - 12 c_{i+1} \right] \quad (\text{IV.12})$$

$$\left(\frac{\partial c}{\partial z} \right)_i = \frac{c_i - c_{i-1}}{h}$$

The above set is applicable for only $i = 1$, where i refers to the grid point number

$$\left(\frac{\partial^2 c}{\partial z^2} \right)_i = - \frac{1}{12h^2} \left[c_{i+2} - 16 c_{i+1} + 30 c_i - 16 c_{i-1} + c_{i-2} \right]$$

$$\left(\frac{\partial c}{\partial z} \right)_i = \frac{0.5 c_{i-2} - 2 c_{i-1} + 1.5 c_i}{h}$$
(IV.13)

The above set is applicable for all the other grid points i.e. $i = 2$ to n (where n is the total number of grid points).

The following matrix differential equation is obtained using the sets (IV.12) and (IV.13).

$$\frac{d}{d\theta} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} = - \frac{1}{12h^2} \begin{bmatrix} (24\alpha+12h) & -12\alpha & & & \\ -(16\alpha+24h) & (30\alpha+18h) & -16\alpha & \alpha & \\ (\alpha+6h) & -(16\alpha+24h) & (30\alpha+18h) & -16\alpha & \alpha \\ & (\alpha+6h) & -(16\alpha+24h) & (30\alpha+18h) & -15\alpha \\ & & (\alpha+6h) & -(15\alpha+24h) & (14\alpha+18h) \end{bmatrix} X$$

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} + \frac{1}{12h^2} \begin{bmatrix} 12(\alpha+h) \\ -(\alpha+6h) \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
(IV.14)

Equation (IV.14) may also be put in the form:

$$\frac{d\underline{c}(\theta)}{d\theta} = - \underline{A}^* \underline{c}(\theta) + \underline{s}'(\theta) \quad (\text{IV.15})$$

The coefficient matrix \underline{A}^* is unsymmetric, but not diagonally dominant and is monotone. Hence it has got all the eigenvalues real, distinct and positive.

The solution to the matrix differential equation (IV.15) is given by (IV.9) and the parameters used are as given in (IV.10).

A summary of results using the backward difference scheme and the central difference scheme for the convective term is given in tables IV.3 and IV.4.

TABLE IV.3

One Dimensional Homogeneous Case
(Using Ordinary Boundary Conditions)

Higher Order Correct Monotone Type Formulations

Summary of Results*. Five Point Grid. Central and Backward Difference formulations for the convective term:

Grid Point Reduced Time	1	3	5
0.2	0.729894 0.746987	0.182635 0.199510	0.013554 -0.011133
0.4	0.884112 0.879907	0.492555 0.515796	0.177966 0.195374
0.6	0.9501 0.932722	0.692501 0.704651	0.416783 0.457964
0.8	0.966106 0.959845	0.812274 0.818074	0.616776 0.654471
1.0	0.979933 0.975450	0.884690 0.887506	0.756546 0.783772

* The first entry in each block refers to the value using central difference scheme for the convective term and the second entry using the backward difference scheme.

TABLE IV.4

One Dimensional Homogeneous Case
(Using Ordinary Boundary Conditions)

Higher Order Correct Monotone Type Formulations

Summary of Results*. Ten Point Grid. Central and Back-
ward Difference formulations for the convective term.

<div>Grid Point Reduced Time</div>	1	3	5	7	9
0.2	0.881985 0.880571	0.558586 0.566481	0.255489 0.259752	0.081094 0.075520	0.017585 0.010342
0.4	0.950738 0.948105	0.793119 0.793709	0.578828 0.583590	0.361881 0.366455	0.201137 0.202516
0.6	0.974442 0.972332	0.888040 0.886336	0.754214 0.755518	0.591811 0.596977	0.446281 0.455248
0.8	0.985539 0.983962	0.935353 0.933153	0.852749 0.852253	0.744875 0.748335	0.641463 0.650337
1.0	0.991533 0.990360	0.961735 0.959560	0.910994 0.909572	0.842425 0.843896	0.774725 0.780750

* The first entry in each block refers to the value using the central difference scheme for the convective term and the second entry using the backward difference scheme.

C. ACCURACY OF THE FINITE DIFFERENCE FORMULATIONS

The accuracy of the central and backward difference scheme for the convective term is tested using an analytical solution to the equation (IV.1) corresponding to the following set of boundary conditions (4):

$$\left. \begin{array}{ll} \text{I.C} & c = 0 \quad \text{at } \theta = 0 \quad 0 \leq z \leq 1 \\ \text{B.C} & c = 0 \quad \text{at } z = 0 \quad \theta > 0 \\ & c = 1 \quad \text{at } z = 1 \end{array} \right\} \quad (\text{IV.16})$$

and the solution is:

$$c = \frac{e^{z/\alpha} - 1}{e^{1/\alpha} - 1} + 2 \sum_{n=1}^{\infty} (-1)^n \frac{n\pi}{(n\pi)^2 + \left(\frac{0.5}{\alpha}\right)^2} \times$$

$$e^{\frac{0.5}{\alpha}(z-1)} \sin(n\pi z) e^{-\left[n^2\pi^2\alpha + \frac{1}{4\alpha}\right]\theta} \quad (\text{IV.17})$$

The equation (IV.1) is discretized using the finite difference sets ((IV.2) and (IV.3)) and ((IV.12) and (IV.13)) corresponding to the boundary conditions set (IV.16).

The matrix differential equations are given by:

- (i) Using central difference scheme for $\frac{\partial c}{\partial z}$.

$$\frac{d}{d\theta} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} = - \frac{1}{12h^2} \begin{bmatrix} 24\alpha & -(12\alpha-6h) & & & \\ -(16\alpha+8h) & 30\alpha & -(16\alpha-8h) & (\alpha-h) & \\ (\alpha+h) & -(16\alpha+8h) & 30\alpha & -(16\alpha-8h) & (\alpha-h) \\ & (\alpha+h) & -(16\alpha+8h) & 30\alpha & -(16\alpha-8h) \\ & & & -(12\alpha+6h) & 24\alpha \end{bmatrix} X$$

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} + \frac{1}{12h^2} \begin{bmatrix} 0 \\ 0 \\ 0 \\ -(\alpha-h) \\ (12\alpha-6h) \end{bmatrix} \quad (IV.18)$$

(ii) Using the backward difference scheme for $\frac{\partial C}{\partial z}$.

$$\frac{d}{d\theta} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} = - \frac{1}{12h^2} \begin{bmatrix} (24\alpha+12h) & -12\alpha & & & \\ -(16\alpha+24h) & (30\alpha+18h) & -16\alpha & \alpha & \\ (\alpha+6h) & -(16\alpha+24h) & (30\alpha+18h) & -16\alpha & \alpha \\ & (\alpha+6h) & -(16\alpha+24h) & (30\alpha+18h) & -16\alpha \\ & & 6h & -(12\alpha+24h) & (24\alpha+18h) \end{bmatrix} X$$

$$\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{bmatrix} + \frac{1}{12h^2} \begin{bmatrix} 0 \\ 0 \\ 0 \\ -\alpha \\ 12\alpha \end{bmatrix} \quad (IV.19)$$

It has been found that the central difference scheme is better as compared to the backward difference scheme up to a value of α slightly greater than one half of the grid spacing. For a value of $\alpha = \frac{h}{2}$, where h is the grid spacing, the central difference scheme fails and the backward difference scheme is applicable at this stage.

The results are represented in the tabular form for various values of α corresponding to the two types of formulations for the convective term.

TABLE IV.5

One Dimensional Homogeneous Case

Summary of Results*. Five Point Grid. Comparison of Central and Backward difference formulations for the convective term

$$\alpha = 0.2$$

Reduced Time \ Grid Point	1	3	5
0.2	0.0005 0.00032 0.00123	0.01968 0.01852 0.03197	0.31639 0.33511 0.38404
0.4	0.00286 0.00289 0.00663	0.0445 0.04513 0.0658	0.37647 0.39128 0.43816
0.6	0.00512 0.00544 0.01067	0.05854 0.05972 0.08313	0.39824 0.41155 0.45837
0.8	0.00655 0.00701 0.01289	0.066 0.06739 0.09194	0.40817 0.42092 0.46782
1.0	0.00736 0.00786 0.01404	0.0699 0.07142 0.09641	0.41312 0.42564 0.47253

* The first entry in each block refers to the value of C calculated by semi-analytical solution using central difference scheme for the convective term, the second entry refers to the value calculated using analytical solution, and the third entry refers to the value using backward difference scheme for the convective term (semi-analytical solution).

TABLE IV.6.

One Dimensional Homogeneous Case

Summary of Results*. Five Point Grid. Comparison of Central and Backward difference formulations for the convective term.

$$\alpha = 0.1$$

Reduced Time \ Grid Point	1	3	5
0.2	0.000024 0.00000 -0.00005	0.00247 0.00068 0.00384	0.07517 0.14032 0.23892
0.4	0.00007 0.00002 0.00033	0.00505 0.00317 0.01247	0.10234 0.17278 0.27589
0.6	0.00011 0.000074 0.00086	0.00653 0.00488 0.01731	0.11278 0.1824 0.28786
0.8	0.000134 0.000124 0.00123	0.00729 0.00579 0.01983	0.11709 0.18601 0.29284
1.0	0.00015 0.000156 0.00145	0.00766 0.00624 0.02114	0.11897 0.18753 0.29518

* The first entry in each block refers to the value of C calculated by semi-analytical solution using central difference scheme for the convective term, the second entry refers to the value using analytical solution, and the third entry refers to the value using backward difference scheme for the convective term. (Semi-analytical solution).

B. EIGENVALUES AND EIGENVECTORS OF A^*

The method used for finding out the eigenvalues and the eigenvectors of a real unsymmetric matrix is described in this section and the detail is available in (34).

The method consists of three steps:-

Step 1:- The given unsymmetric matrix A^* is first reduced to the Hessenberg form using Householder's method:

$$\begin{aligned} \text{Let } \underline{A}_0 &= \underline{A}^*, \text{ the original matrix} \\ \text{and } \underline{A}_r &= \underline{P}_r \underline{A}_{r-1} \underline{P}_r \end{aligned} \quad (\text{IV.20})$$

Then after $(n-2)$ steps.

$$\underline{A}_{n-2} = \underline{H} \quad (\text{IV.21})$$

where \underline{H} = The Hessenberg matrix.

The other symbols are as given below:

$$\left. \begin{aligned} \underline{P}_r &= \underline{I} - 2 \frac{\underline{\omega}_r \underline{\omega}_r^T}{\underline{\omega}_r^T \underline{\omega}_r} \\ &= \underline{I} - \frac{\underline{u}_r \underline{u}_r^T}{\underline{u}_r^T \underline{u}_r} \\ \text{and } u_{ir} &= 0 \quad (i = 1 \text{ to } r) \\ u_{r+1,i} &= a_{r+1,r} \mp s \quad i = (r+2) \text{ to } n \\ u_{i,r} &= a_{i,r} \\ s_r &= \left(\sum_{i=r+1}^n (a_{i,r}^2) \right)^{1/2} \\ 2k_r^2 &= s_r^2 \mp a_{r+1,r} s_r \end{aligned} \right\} \quad (\text{IV.22})$$

The sign is chosen to be that of $a_{r+1,r}$.

Step 2:- Once the Hessenberg matrix is derived, Newton's method is used to find out the roots of the characteristic equation. First $F(z)$ and $F'(z)$ are found, where $F(z)$ is the value of the characteristic equation and $F'(z)$ is the value of the first derivative. Then a new estimate of z is found from the equation (IV.23).

$$z_{k+1} = z_k - \frac{F(z_k)}{F'(z_k)} \quad (\text{IV.23})$$

If the value of z has converged to within a given tolerance limit

$$((z_{k+1} - z_k) / \text{Max}(z_{k+1}, z_k)) \leq 10^{-6}$$

the value of z is taken to be the root.

If the first r zeros have been found, the program suppresses these zeros by computing:

$$g_r(z) = F(z) / \prod_{i=1}^r (z - \lambda_{ii}) \quad (\text{IV.24})$$

$$g'_r(z) = \left[F'(z) / F(z) - \sum_{i=1}^r 1 / (z - \lambda_{ii}) \right] \times g_r(z)$$

where λ_{ii} are the first r eigenvalues. (IV.25)

Step 3:- Once the eigenvalues are found within the prescribed tolerance limit, the next step is to find the eigenvectors. For finding out the eigenvectors the matrix $(\underline{A} - \lambda_{ii} \underline{I})$ is triangularized by Gaussian elimination with complete pivoting. The eigenvector is found by back substitution

The eigenvectors are distinct. For a root of multiplicity m , which has $r < m$ distinct eigenvectors associated with it, the remaining $(m - r)$ eigenvectors are returned as null vectors.

V. SUMMARY AND CONCLUSIONS

1. A general solution of the dispersion model equation in its semi-discrete form has been developed. The discretization of the space derivatives of the parabolic partial differential equation gives rise to a set of ordinary differential equations. The coefficient matrix of this system is diagonally dominant and unsymmetric. For some problems the coefficient matrix has been converted to the real symmetric form using similarity transformation. The various methods of linear algebra and matrix theory have been made use of in getting a general solution to the problem. A closed form of solution has been obtained in terms of spatial properties distribution, the eigenvalues and the eigenvectors of the coefficient matrix. The solution has been tested on various problems using two sets of boundary conditions. To get an overall idea about the accuracy of the solution obtained the results of a lower point grid are derived from those of a higher point grid using interpolation and compared with the results obtained using the semi-analytical method.
2. The solution to the one dimensional homogeneous case has also been obtained using the higher order correct monotone type approximations. The coefficient matrix for this case is unsymmetric, monotone and may or may not be diagonally dominant. In many problems of this type the convective term is large and for such cases the second order correct backward difference scheme for the convective term is recommended. The accuracy

of the central and backward difference formulations for the convective term is tested by taking an analytical solution (4) corresponding to a simple set of boundary conditions. The comparison of the difference between the analytical and semi-analytical values suggests, that the central difference scheme for the convective term is better as compared to the backward difference scheme up to a value of α slightly greater than one half of the grid spacing. The central difference scheme fails for a value of $\alpha = \frac{h}{2}$, where h is the grid spacing and for the values of $\alpha < \frac{h}{2}$, the backward difference scheme is applicable.

3. The main objective of this work is to get the solution in the time domain. The solutions in the transformed domain have been attempted in the past but the present approach is better as compared to the Laplace transform approach. Three different input signals have been tried i.e. the time dependent boundary conditions, to correlate this work with the previous work. The three input signals are:

- *(a) Step Input
- (b) Sine Wave Input (Frequency response)
- (c) Square Wave Input

The output response curves have been obtained for the above cases using ordinary and Danckwerts boundary conditions. The plots of the output response curves show that there is a significant difference in the model using the two sets of boundary conditions. Shemilt and Krishnaswamy (26) report in their work that there is no appreciable difference between the

* The details results are available in Appendix F.

B.C(i) : ORDINARY BOUNDARY CONDITIONS
B.C(ii) : DANCKWERTS BOUNDARY CONDITIONS

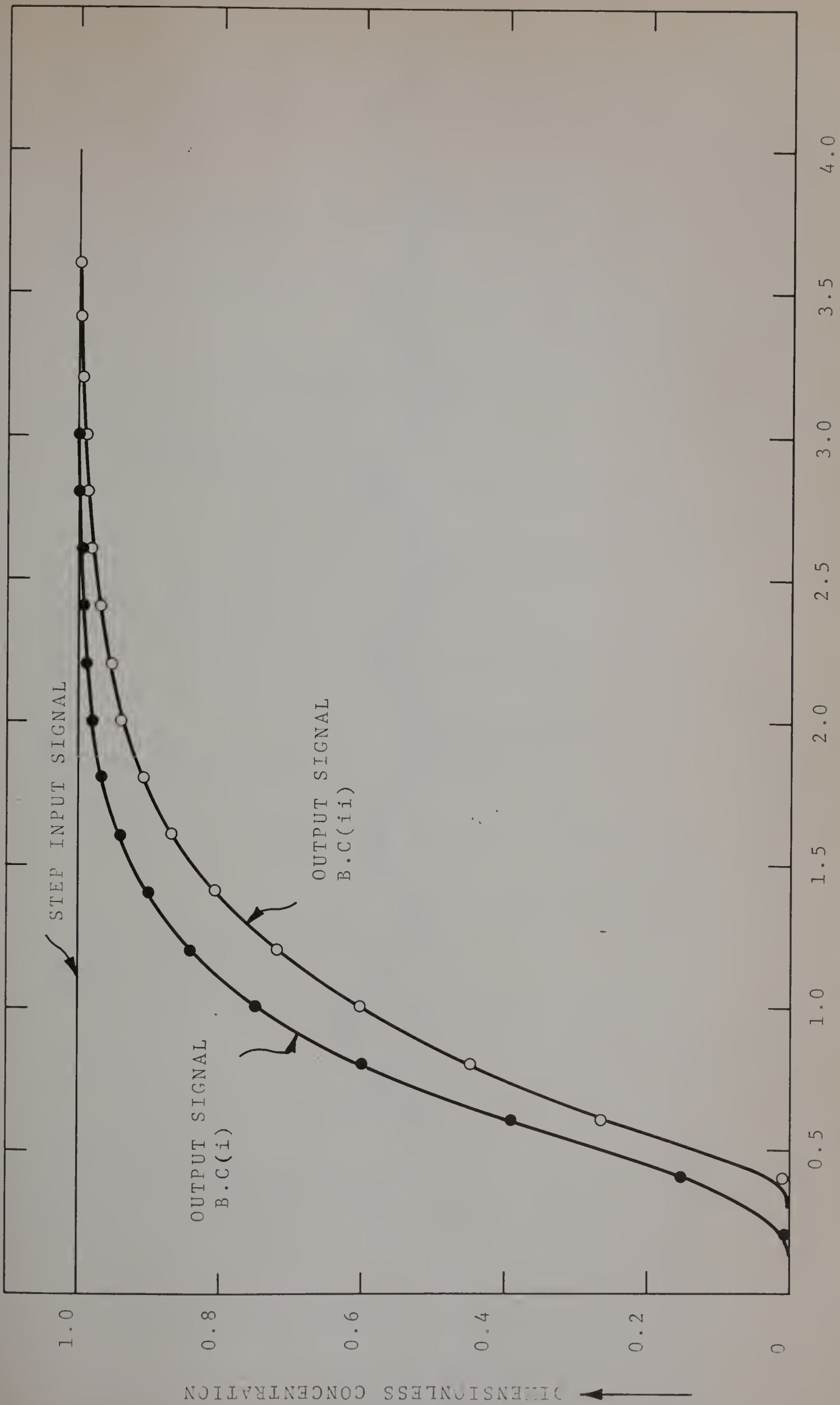
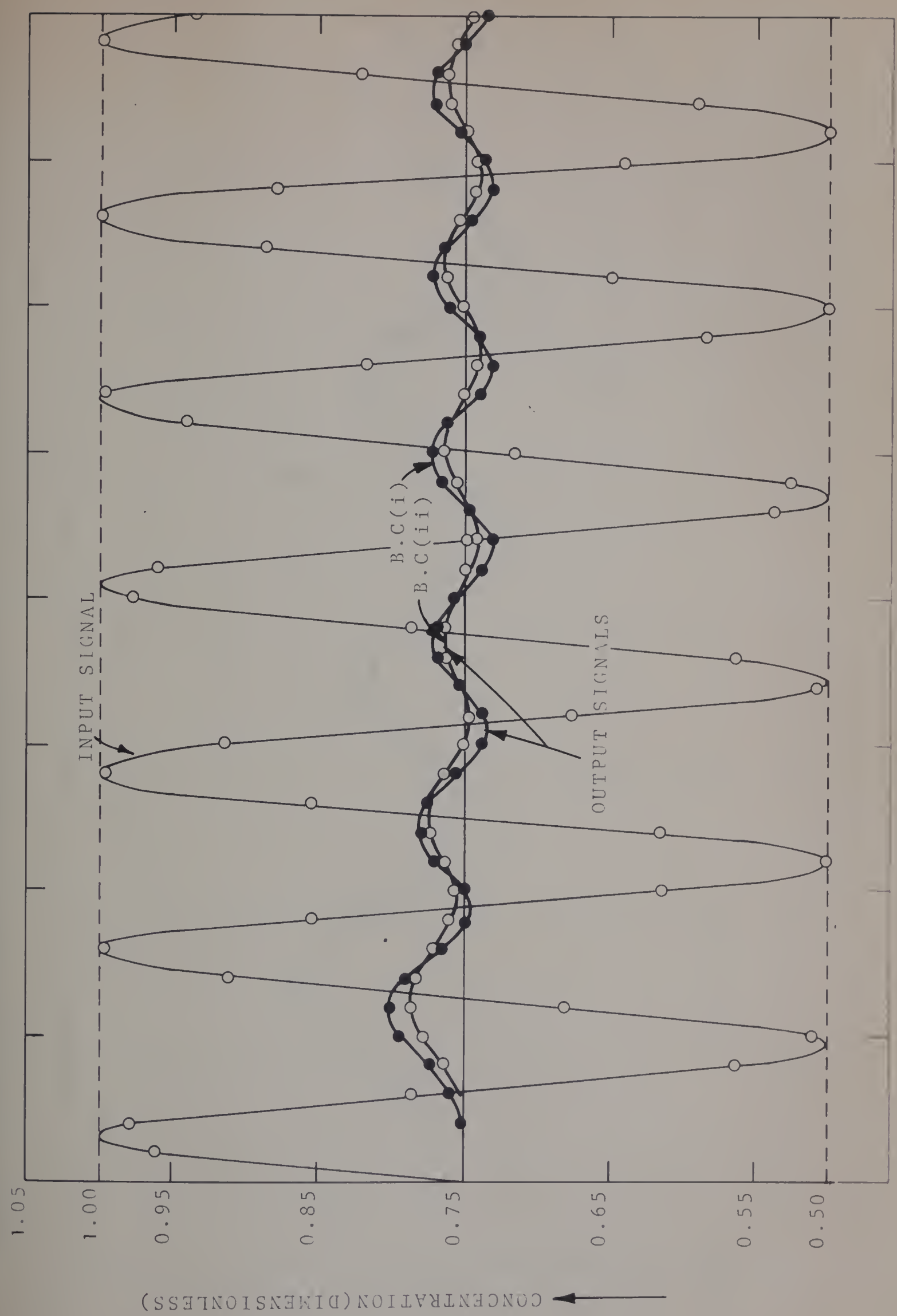


FIGURE V-a STEP INPUT OUTPUT RESPONSE CURVES

B.C(ii) DANCVERTS BOUNDARY CONDITIONS O



0.5 1.0 1.5 2.0 2.5 3.0 4.0

FIGURE V-6 SINE WAVE INPUT OUTPUT RESPONSE CURVES

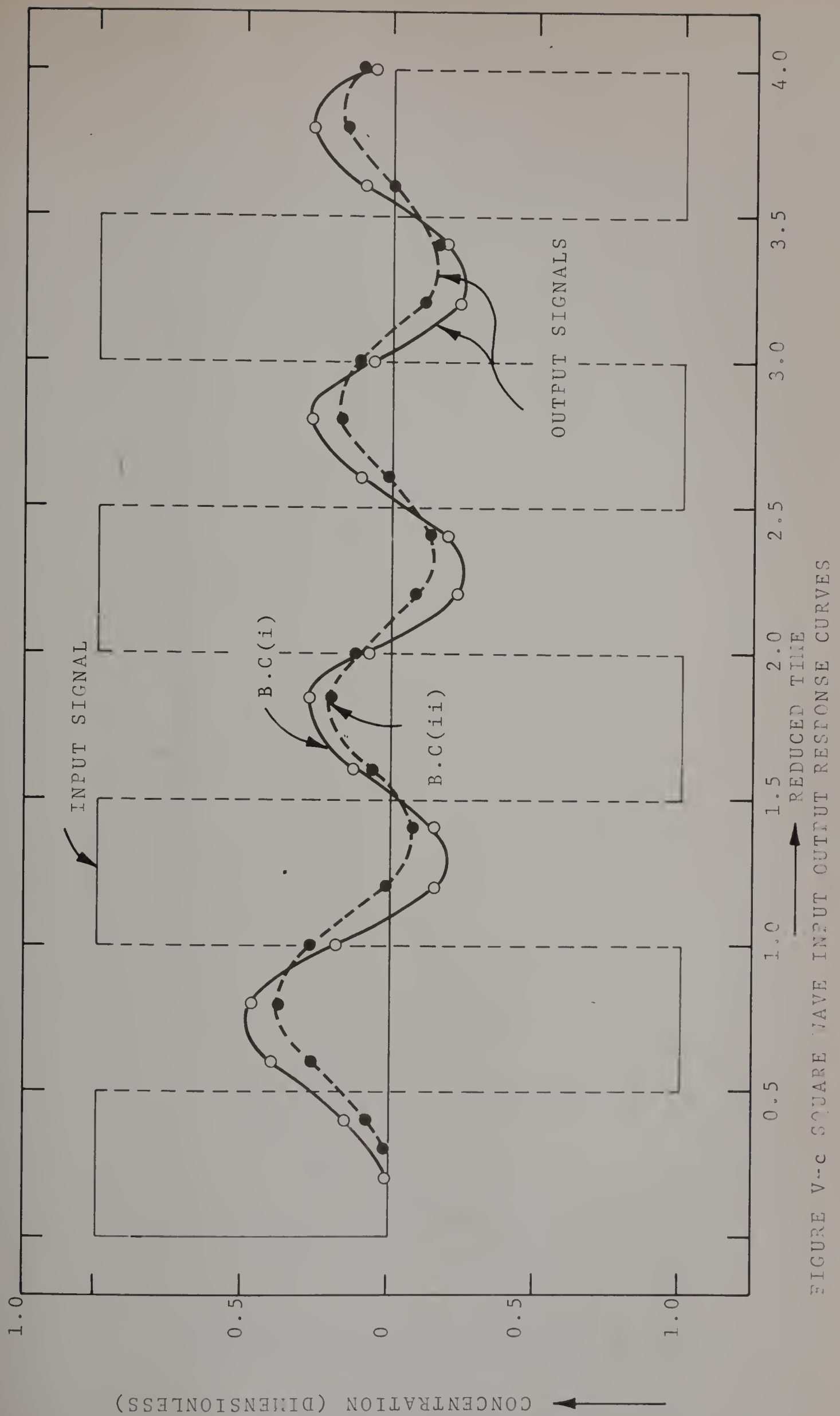


FIGURE V-c SQUARE WAVE INPUT OUTPUT RESPONSE CURVES

B.(i). ORDINARY BOUNDARY CONDITIONS
B.C(ii). PANKWERTS BOUNDARY CONDITIONS

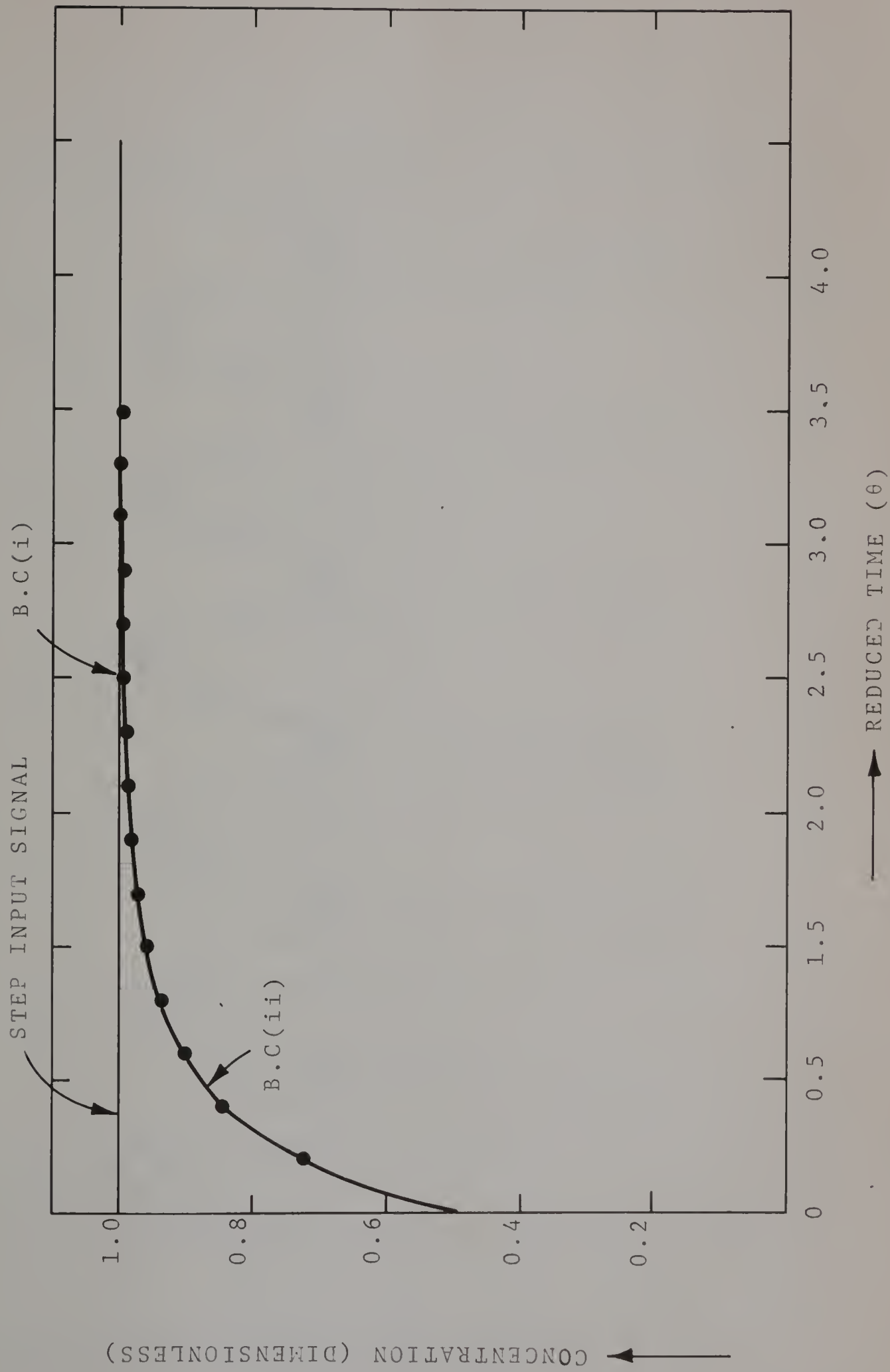


FIGURE V-d STEP INPUT DIFFERENCE IN CONCENTRATION AT THE FIRST BOUNDARY
USING B.C(ii) & B.C(i)

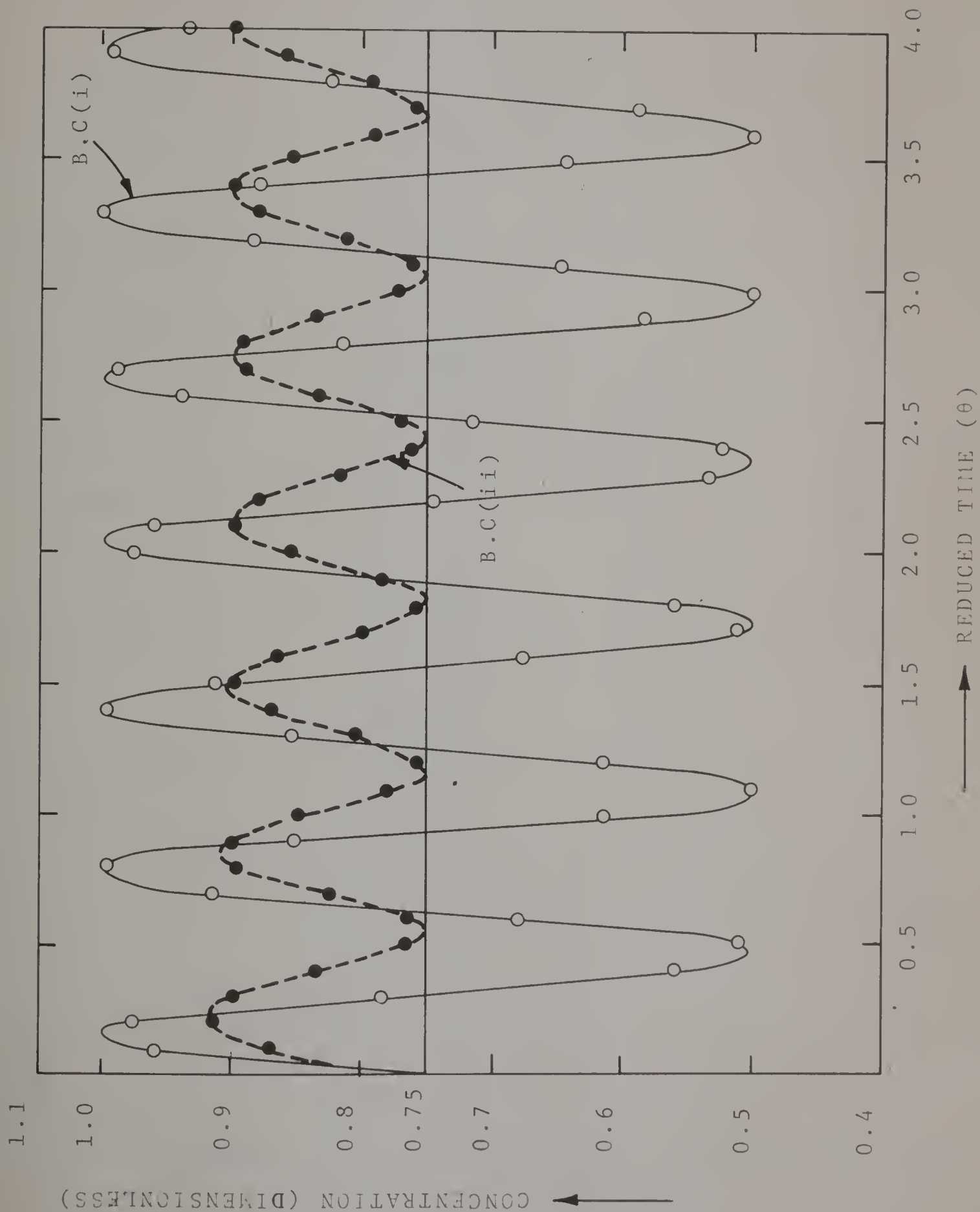


FIGURE V-e SINE WAVE INPUT
CONCENTRATION DIFFERENCE AT THE FIRST BOUNDARY USING B.C(i) & B.C(ii)

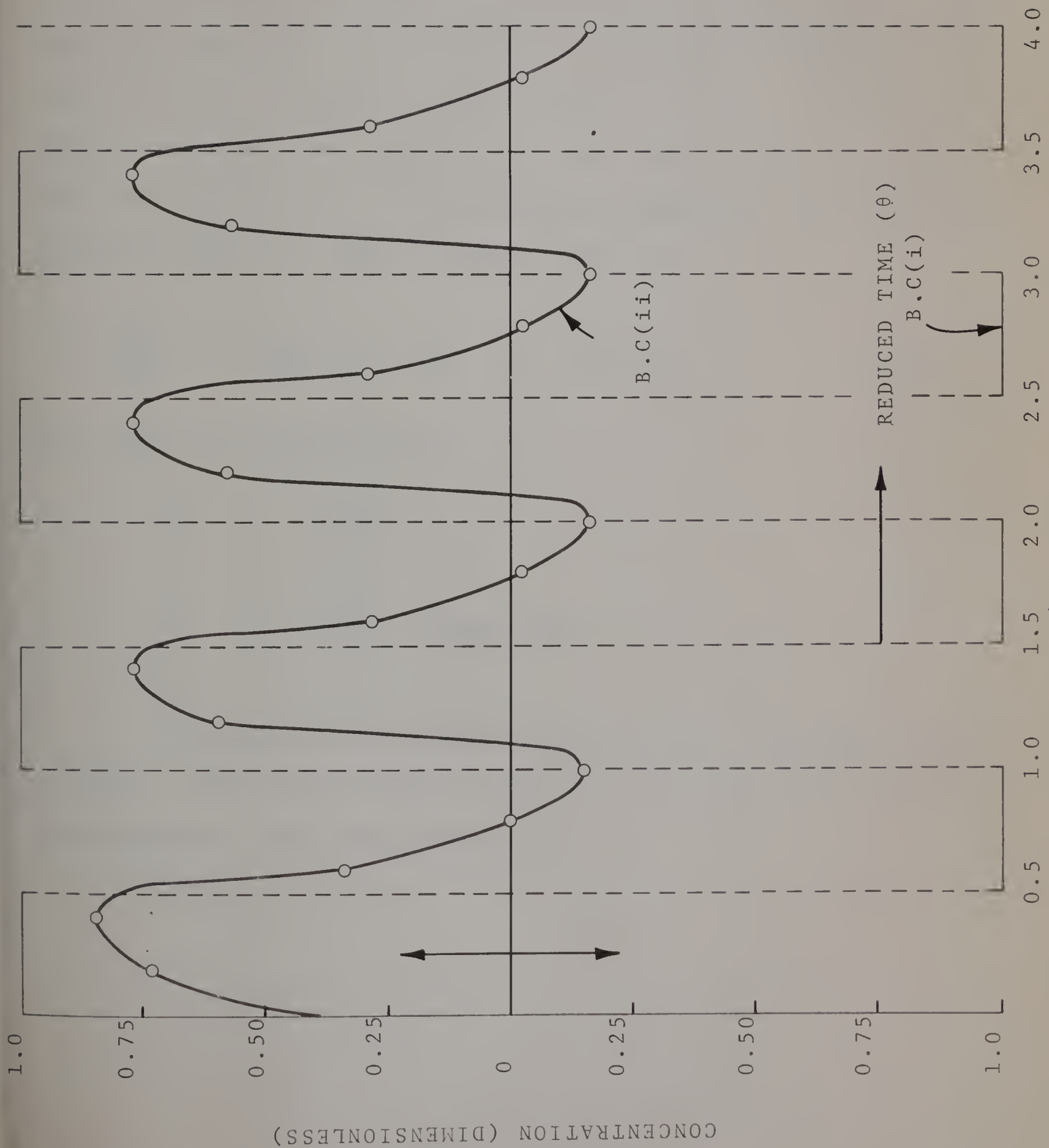


FIGURE V-f SQUARE WAVE INPUT SIGNAL
DIFFERENCE IN CONCENTRATIONS AT THE FIRST BOUNDARY USING B.C(i) & B.C(ii)

output response curves in the transformed domain using the ordinary and Danckwerts boundary conditions. The difference in the two sets of boundary conditions is clearly evident from the figures (V-d, e, f) respectively.

4. A simpler model has also been derived corresponding to the frequency response using quasilinearization (11). The data are generated corresponding to different values of ω , where ω is the frequency (Input signal is $0.75 + 0.25 \sin \omega\theta$), using semi-analytical solution. Four sets of data were used for the calculation of the best fit parameters. The data are given in table V.1 and the model used is:-

$$\frac{d^2c}{d\theta^2} + C^* \frac{dc}{d\theta} + B.C = Bf(\theta-A) \quad (V.1)$$

The best fit constants are:-

$$\left. \begin{array}{lcl} C^* & = & 6.54 \\ B & = & 10.62 \\ A & = & 0.187 \text{ (Time Delay)} \end{array} \right] \quad (V.2)$$

The sum of the squares of the errors was found to be 0.00035. Hence this simpler model can represent the original complex model quite satisfactorily.

TABLE V.1

One Dimensional Homogeneous Case

Input Signal Sine Wave Input

* Data used for the calculation of Best Fit Parameters using Quasilinearization

Reduced Time θ	Output Signal			
	$\omega = 0.1$	$\omega = 1.0$	$\omega = 5.0$	$\omega = 10.0$
0.5	0.752267	0.760247	0.788839	0.795385
1.0	0.759911	0.825010	0.842310	0.752342
1.5	0.770823	0.909480	0.685289	0.738393
2.0	0.782802	0.968236	0.809963	0.757490
2.5	0.795050	0.978149	0.740429	0.773722
3.0	0.807298	0.934066	0.718791	0.761064
3.5	0.819441	0.845946	0.820425	0.736795
4.0	0.831428	0.735108	0.678430	0.735424
4.5	0.843220	0.628611	0.804073	0.758835
5.0	0.854788	0.552505	0.744679	0.773463

5. The various two dimensional models have also been investigated in detail. The most complicated model taking into account the packed bed velocity profile and the variation of the radial dispersion coefficient with radial position has been tried but the eigenvalues did not converge to the actual value even within 90 iterations and corresponding to a convergence limit of 0.001. Then simpler models have also been tried i.e. (i) flat velocity profile and the variation of radial dispersion group with radial positions; (ii) flat velocity profile and using an average value of the radial dispersion group. The weighted average of the two dimensional model results has also been compared with the simple one dimensional model results for three different sets of the ratio (d_p/d_T) i.e. Particle diameter/Tube diameter. The results indicate that the simple one dimensional model represents fairly well the two dimensional nonhomogeneous model up to a variation of -37.0 to 50% in the radial Peclet number and $(\frac{d_p}{d_T}) = 0.075$. With the increase of this ratio, the agreement in the two models is not so good. For a variation of -48.0 to 60.0% in the radial Peclet number and $\frac{d_p}{d_T} = 0.125$, the agreement is not good with the higher values of time elapsed. The agreement between the two dimensional homogeneous model (using an average value of the dispersion group), and the one dimensional model is found to be quite good. The summarized results for two sets of $\frac{d_p}{d_T}$ are shown in tables V.2 and V.3.

N.B. The detailed results for one set of $\frac{d_p}{d_T}$ are available in Appendices C and C1.

TABLE V.2

Two Dimensional Models

Summary of Results^{*1}: Comparison of one dimensional and two dimensional models.

^{*2} Pe. No. Variaton = -48 to 60%

$\frac{dP}{dT} = 0.125$	Two Dimensional Homogeneous Model			Two Dimensional Nonhomogeneous Model		
<div>Grid Point Reduced Time</div>	1	3	5	1	3	5
0.2	0.73145	0.19183	0.02455	0.73152	0.19224	0.02458
	0.73145	0.19184	0.02455	0.73145	0.19184	0.02455
	0.00000	-0.00001	0.00000	0.00007	0.0004	0.00003
0.4	0.88328	0.48818	0.18226	0.88361	0.49000	0.18277
	0.88329	0.48820	0.18227	0.88329	0.48820	0.18227
	-0.00001	-0.00002	-0.00001	0.00032	0.0018	0.0005
0.6	0.93902	0.68561	0.40472	0.93964	0.68898	0.40629
	0.93904	0.68567	0.40475	0.93904	0.68567	0.40475
	-0.00002	-0.00006	-0.00003	0.0006	0.00331	0.00154
0.8	0.96525	0.80577	0.59816	0.96610	0.81042	0.60105
	0.96527	0.80585	0.59823	0.96527	0.80585	0.59823
	-0.00002	-0.00008	-0.00007	0.00083	0.00457	0.00282
1.0	0.97926	0.87915	0.73856	0.98028	0.8848	0.74268
	0.97929	0.87925	0.73865	0.97929	0.87925	0.73865
	-0.00003	-0.00010	-0.00009	0.00099	0.00555	0.00403

^{*1} The first entry in each block refers to the weighted average of C calculated from the generated values of the two dimensional model using semi-analytical solution i.e. n the second entry refers to the value of C corresponding to one dimensional homogeneous model and the third entry represents the difference between the two values.

$$(C = \frac{\sum_{i=1}^n C_i R_i}{\sum_{i=1}^n R_i}),$$

^{*2} Pe. No. Variation = ((Point Pe.No. - Average Pe.No.) / (Average Pe. No.) x 100.

TABLE V.3

Two Dimensional Models

Summary of Results^{*1}: Comparison of one dimensional and two dimensional models.

^{*2} Peclet No. Variation = -37 to 50%

$\frac{dP}{dT} = 0.075$	Two Dimensional Homogeneous Model			Two Dimensional Nonhomogeneous Model		
Grid Point Reduced Time	1	3	5	1	3	5
0.2	0.73145	0.19184	0.02455	0.73144	0.19183	0.02455
	0.73145	0.19184	0.02455	0.73145	0.19184	0.02455
	0.00000	0.00000	0.00000	-0.00001	-0.00001	0.00000
0.4	0.88329	0.48820	0.18227	0.88327	0.48820	0.18226
	0.88329	0.48820	0.18227	0.88329	0.48220	0.18227
	0.00000	0.00000	0.00000	-0.00002	0.00000	-0.00001
0.6	0.93904	0.68566	0.40475	0.93902	0.68563	0.40472
	0.93904	0.68567	0.40475	0.93904	0.68567	0.40475
	0.00000	-0.00001	0.00000	-0.00002	-0.00004	-0.00003
0.8	0.96527	0.80584	0.59822	0.96525	0.80579	0.59817
	0.96527	0.80585	0.59823	0.96527	0.80585	0.59823
	0.00000	-0.00001	-0.00001	-0.00002	-0.00006	-0.00006
1.0	0.97929	0.87924	0.73864	0.97926	0.87919	0.73857
	0.97929	0.87925	0.73865	0.97929	0.87925	0.73865
	0.0000	-0.00001	-0.00001	-0.00003	-0.00006	-0.00008

^{*1} The first entry in each block refers to the weighted average of C calculated from the generated valued of the two dimensional model using semi-analytical solution i.e.
$$C = \frac{\sum_{i=1}^n C_i R_i}{\sum_{i=1}^n R_i}$$
 the second entry refers to the value of C corresponding to one dimensional homogeneous models and the third entry represents the difference between the two values.

^{*2} Pe. No. Variation = ((Point Pe.No. - Average Pe.No.)/Average Pe.No.) x 100

Hence it is concluded that the solution developed in this thesis is capable of handling wide varieties of initial and boundary conditions. It can also handle all one dimensional problems and many two dimensional homogeneous or nonhomogeneous media (provided, of course, the properties of the media are independent of the dependent variable and time) problems.

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A P P E N D I C E S

A. RELATED TOPICS OF MATRIX ALGEBRA

The proofs of the various theorems of matrix algebra given here have been taken from the standard text books of numerical analysis such as,

Lapidus L. Digital Computation for Chemical Engineers.

THEOREM 1. If a matrix undergoes a similarity transformation, the eigenvalues remain unchanged but the eigenvectors are changed.

If a matrix \underline{A} is formed from a given matrix \underline{A}^* by

$$\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D} \quad (\text{A.1})$$

where \underline{D} is a regular matrix, then \underline{A}^* is said to undergo a similarity transformation.

The proof is given in two parts.

(a) Eigenvalues of \underline{A} & \underline{A}^* are same

i.e. The characteristic equation is invariant during such transformation.

$$\det (\underline{A} - \lambda \underline{I})$$

$$= \det \left[(\underline{D}^{-1} \underline{A}^* \underline{D} - \lambda \underline{I}) \right]$$

$$= \det \left[(\underline{D}^{-1} \underline{A}^* \underline{D} - \lambda \underline{I}) \right]$$

$$= \det \left[\underline{D}^{-1} (\underline{A}^* \underline{D} - \lambda \underline{I} \underline{D}) \right]$$

$$= \det \left[\underline{D}^{-1} (\underline{A}^* - \lambda \underline{I}) \underline{D} \right]$$

$$\begin{aligned} &= \det \underline{D}^{-1} \cdot \det (\underline{A}^* - \lambda \underline{I}) \cdot \det \underline{D} \\ &= \det (\underline{A}^* - \lambda \underline{I}) \end{aligned}$$

$$\text{Hence } \det (\underline{A} - \lambda \underline{I}) = \det (\underline{A}^* - \lambda \underline{I}) \quad (\text{A.2})$$

$$(\because \det \underline{D}^{-1} \cdot \det \underline{D} = \det (\underline{D}^{-1} \underline{D}) = 1).$$

Hence the eigenvalue of \underline{A} and \underline{A}^* are same.

(b) Eigenvectors of \underline{A} and \underline{A}^* are not same.

Let \underline{u} be an eigenvector of \underline{A}^*

and \underline{v} be an eigenvector of \underline{A}

both with the same eigenvalue λ

Then

$$\underline{A}^* \underline{u} = \lambda \underline{u} \quad (\text{A.3})$$

and

$$\underline{A} \underline{v} = \lambda \underline{v} \quad (\text{A.4})$$

But

$$\underline{A} = \underline{D}^{-1} \underline{A}^* \underline{D} \quad (\text{A.5})$$

Consequently

$$(\underline{D}^{-1} \underline{A}^* \underline{D}) \underline{v} = \lambda \underline{v} \quad (\text{A.6})$$

Premultiplication by \underline{D} gives

$$\underline{A}^* (\underline{D} \underline{v}) = \lambda (\underline{D} \underline{v}) \quad (\text{A.7})$$

Comparing equations (A.3) and (A.7) clearly indicates:

If \underline{v} is an eigenvector of \underline{A} , then $\underline{D} \underline{v}$ is an eigenvector of \underline{A}^* .

Hence $\underline{u} = \underline{D} \underline{v}$ is an eigenvector of \underline{A}^* where \underline{v} is the eigenvector of \underline{A} .

THEOREM 2. The eigenvalues of a real, symmetric matrix \underline{A} ($\underline{D}^{-1}\underline{A}^*\underline{D}$) are real, distinct and positive.

The proof is given in three steps:-

(i) The Eigenvalues of \underline{A} are real:

Let λ_1 be a complex eigenvalue of \underline{A} . Then, since \underline{A} is real, it follows from the characteristic equation

$$\det (\underline{A} - \lambda \underline{I}) = 0 \quad (\text{A.8})$$

that the complex conjugate λ_1^* of any complex root λ_1 is also an eigenvalue. This implies that the corresponding eigenvectors \underline{u}_1 and \underline{u}_1^* are complex.

Since λ_1 is an eigenvalue and \underline{u}_1 is an eigenvector, the following relation is satisfied:

$$\underline{A} \underline{u}_1 = \lambda_1 \underline{u}_1 \quad (\text{A.9})$$

also

$$\underline{A} \underline{u}_1^* = \lambda_1^* \underline{u}_1^* \quad (\text{A.10})$$

Premultiplication of equation (A.9) \underline{u}_1^{*T} and equation (A.10) by \underline{u}_1^T gives:

$$\underline{u}_1^{*T} \underline{A} \underline{u}_1 = \lambda_1 \underline{u}_1^{*T} \underline{u}_1 \quad (\text{A.11})$$

and

$$\underline{u}_1^T \underline{A} \underline{u}_1^* = \lambda_1^* \underline{u}_1^T \underline{u}_1^* \quad (\text{A.12})$$

Since \underline{A} is a symmetric matrix, the left hand sides of equations (A.11) and (A.12) are equal.

This gives:

$$(\lambda_1 - \lambda_1^*) (\underline{u}_1^T \underline{u}_1^*) = 0 \quad (A.13)$$

$$\text{or } \lambda_1 = \lambda_1^*$$

But this is contrary to the assumption. Hence all the eigenvalues of a real and symmetric matrix \underline{A} are real.

(ii) The matrix \underline{A} has n distinct eigenvalues.

Proof: Order the eigenvalues of \underline{A} in such a way that

$$|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n| \quad (A.14)$$

and consider the p^{th} compound $A(p)$ of the matrix \underline{A} ($p = 1, 2, \dots, n$) i.e. the matrix whose elements are $(p \times p)$ minor determinants of \underline{A} , indexed in some order. The characteristic numbers i.e. eigenvalues of $A^{(p)}$ are the various products of eigenvalues of \underline{A} , taken p at a time:

$$\lambda_1 \lambda_2 \dots \lambda_p, \lambda_1 \lambda_2 \dots \lambda_{p-1} \lambda_{p+1} \dots \quad (A.15)$$

By hypothesis there is an integer q so that $A^{(q)}$ is totally positive. From $A_{(p)} \cdot A_{(p)} = (A^2)_{(p)}$, we see that $A_{(p)}^{(q)}$ is the p^{th} compound of A^q and is therefore totally positive. On the other hand $A_{(p)}$ is non negative ($A_{(p)} > 0$). Thus $A_{(p)}$ is actually an irreducible non negative matrix and so is a primitive matrix. By the theorem of Frobenius (15, page 65) we conclude:

$$\left. \begin{aligned} \lambda_1 \lambda_2 \cdots \lambda_p &> 0 \quad (p = 1, 2, \dots, n) \\ \lambda_1 \lambda_2 \cdots \lambda_p &> \lambda_1 \lambda_2 \cdots \lambda_{p-1} \lambda_{p+1} \quad (p = 1, 2, \dots, n-1) \end{aligned} \right] \quad (A.16)$$

So the inequalities (A.16) imply

$$\lambda_1 > \lambda_2 > \lambda_3 > \dots > \lambda_n$$

Hence all the eigenvalues of \underline{A} are distinct.

(iii) The eigenvalues of \underline{A} are positive numbers.

Proof: Consider a five point grid and the typical coefficient matrix associated with it is

$$\underline{A} = \begin{bmatrix} 12.1 & 5.4 & & & \\ 5.4 & 12.1 & 5.4 & & \\ & 5.4 & 12.1 & 5.4 & \\ & & 5.4 & 12.1 & 5.4 \\ & & & 5.4 & 8.8 \end{bmatrix} \quad (A.17)$$

Any matrix \underline{A} is said to be diagonally dominant if

$$|a_{ii}| \geq \sum_{j=1}^n |a_{ij}|, \quad i = 1 \text{ to } n \quad (A.18)$$

The condition as given by (A.18) is seen to be true in the present case. The matrix \underline{A} is said to be irreducibly diagonally dominant if the inequality holds for

at least one i . This can also be verified in the present case. Since the diagonal elements of \underline{A} are positive, the eigenvalues of \underline{A} are also positive as given in (29).

Hence this also establishes that the matrix \underline{A} is a positive definite matrix.

THEOREM 3. A real, symmetric matrix \underline{A} of order n has n linearly independent and mutually orthogonal eigenvectors.

The proof of this theorem is presented in two parts.

(i) To prove that the eigenvectors associated with distinct eigenvalues are orthogonal.

Consider two distinct eigenvalues λ_1 and λ_2 and the associated eigenvectors \underline{u}_1 and \underline{u}_2 . Then,

$$\underline{A} \underline{u}_1 = \lambda_1 \underline{u}_1 \quad (\text{A.19})$$

and
$$\underline{A} \underline{u}_2 = \lambda_2 \underline{u}_2 \quad (\text{A.20})$$

The scalar product of equation (A.19) with \underline{u}_2 and of equation (A.20) with \underline{u}_1 are:

$$\underline{u}_2^T \underline{A} \underline{u}_1 = \lambda_1 \underline{u}_2^T \underline{u}_1 \quad (\text{A.21})$$

and
$$\underline{u}_1^T \underline{A} \underline{u}_2 = \lambda_2 \underline{u}_1^T \underline{u}_2 \quad (\text{A.22})$$

Since matrix \underline{A} is symmetric

$$\underline{u}_2^T \underline{A} \underline{u}_1 = \underline{u}_1^T \underline{A} \underline{u}_2 \quad (\text{A.23})$$

or
$$(\lambda_1 - \lambda_2) (\underline{u}_1^T \underline{u}_2) = 0 \quad (\text{A.24})$$

λ_1 and λ_2 are two distinct eigenvalues,

$\therefore \underline{u}_1^T \underline{u}_2$ must be zero in order that equation (A.24) is satisfied.

Hence the eigenvectors associated with distinct eigenvalues are orthogonal.

(ii) To prove that there exists k linearly independent, and orthogonal eigenvectors associated with λ_1 where λ_1 is a root of multiplicity k .

Let $\lambda_1 = \lambda_2 = \dots = \lambda_k$, but $\lambda_i \neq \lambda_1$
for $i = k + 1, \dots, n$.

The proof is by induction

$$\text{Let } \underline{A}_2 = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} \underline{a}^{(1)} \\ \underline{a}^{(2)} \end{bmatrix} \quad (\text{A.25})$$

be a symmetric matrix.

Let λ_1 and \underline{u}_1 be a set of associated eigenvalues and eigenvectors, then

$$\left. \begin{aligned} \underline{A}_2 \underline{u}_1 &= \lambda_1 \underline{u}_1 \quad \text{or} \\ \underline{a}^{(1)} \underline{u}_1 &= \lambda_1 u_{11} \quad \text{and} \quad \underline{a}^{(2)} \underline{u}_1 = \lambda_1 u_{21} \end{aligned} \right] \quad (\text{A.26})$$

Let \underline{T}_2 be an orthogonal matrix, one of whose columns is \underline{u}_1 . Let the other column be \underline{u}_2 . In matrix notation

$$\underline{T}_2 = [\underline{u}_1, \underline{u}_2]$$

It is required to show that

$$\underline{T}_2^T \underline{A}_2 \underline{T}_2 = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \quad (\text{A.26})$$

where λ_1 and λ_2 are the eigenvalues of \underline{A}_2 , not necessarily distinct.

Evaluating the left hand side of equation (A.26) to give

$$\underline{T}_2^T \underline{A}_2 \underline{T}_2 = \begin{bmatrix} \lambda_1 & C_{12} \\ 0 & C_{22} \end{bmatrix}$$

It is easily shown that $C_{12} = 0$ for

$$\left[\underline{T}_2^T \underline{A}_2 \underline{T}_2 \right]^T = \underline{T}_2^T \underline{A}_2^T (\underline{T}_2^T)^T = \underline{T}_2^T \underline{A}_2 \underline{T}_2 \quad (\text{A.27})$$

or $\underline{T}_2^T \underline{A}_2 \underline{T}_2$ is a symmetric matrix. Hence C_{12} has to be zero. Also, since the eigenvalues of $\underline{T}_2^T \underline{A}_2^T$ and \underline{A}_2 are the same, it can be easily shown that $C_{22} = \lambda_2$. This also proves that \underline{u}_2 is the second eigenvector.

The n^{th} order case is now proved by induction

Assume that for each k , $k = 1, 2, \dots, n$ an orthogonal matrix \underline{T}_k can be found which reduces \underline{A}_k to the diagonal form. It is to be proved if the above is valid for n , it is valid for $n + 1$ also.

$$\text{Let } \underline{A}^{(n+1)} = (a_{ij}) = \begin{bmatrix} \underline{a}^{(1)} \\ \underline{a}^{(2)} \\ \vdots \\ \underline{a}^{(n+1)} \end{bmatrix} \quad (\text{A.28})$$

Let λ_1 and \underline{u}_1 be the set of associated eigenvalue and eigenvector. An orthogonal matrix T_1 is formed with \underline{u}_1 as its first column. Let T_1 be

$$T_1 = [\underline{u}_1, \underline{u}_2, \dots, \underline{u}_{n+1}]$$

Now
 $\underline{A}_{n+1} T_1 =$

$$\begin{bmatrix} \underline{a}^{(1)} \underline{u}_1 & \dots & \dots & \dots & \underline{a}^{(1)} \underline{u}_{n+1} \\ \vdots & & & & \vdots \\ \underline{a}^{(n+1)} \underline{u}_1 & \dots & \dots & \dots & \underline{a}^{(n+1)} \underline{u}_{n+1} \end{bmatrix}$$

=

$$\begin{bmatrix} \lambda_1 u_{11} & \underline{a}^{(1)} \underline{u}_2 & \dots & \dots & \underline{a}^{(1)} \underline{u}_{(n+1)} \\ \vdots & \vdots & & & \vdots \\ \lambda_1 u_{n+1,n+1} & \underline{a}^{(n+1)} \underline{u}_2 & \dots & \dots & \underline{a}^{(n+1)} \underline{u}_{(n+1)} \end{bmatrix} \quad (\text{A.29})$$

Since \underline{T}_1 is an orthogonal matrix

$$\begin{matrix} \underline{T}_1^T \underline{A}_{(n+1)} \\ \underline{T}_1 \end{matrix} = \begin{bmatrix} \lambda_1 & a_{12} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_{1,n+1} \\ 0 & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ 0 & & & & & & & & & & & & & \end{bmatrix} \quad (A.30)$$

Since $\underline{T}_1^T \underline{A}_{n+1} \underline{T}_1$ is symmetric, $a_{12} = a_{13} = \dots = a_{1,n+1} = 0$.

$$\therefore \underline{T}_1^T \underline{A}_{(n+1)} \underline{T}_1 = \begin{bmatrix} \lambda_1 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & & & & & & & & & & & & & \\ 0 & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ \cdot & & & & & & & & & & & & & \\ 0 & & & & & & & & & & & & & \end{bmatrix} \quad (A.31)$$

Now the eigenvalues of \underline{A}_n must be the same as the other eigenvalues of $\underline{A}_{(n+1)}$.

The theory of induction is employed at this stage. Let \underline{T}_n be the orthogonal matrix which reduces \underline{A}_n to the diagonal form.

$$\text{Let } \underline{S}_{n+1} = \begin{bmatrix} 1 & 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & & & & & & & \\ \vdots & & & & & & & \\ \vdots & & & & & & & \\ \vdots & & & & & & & \\ \vdots & & & & & & & \\ \vdots & & & & & & & \\ 0 & & & & & & & \end{bmatrix} \quad (A.32)$$

which is also orthogonal. Now

$$\underline{S}_{n+1}^T (\underline{T}_1^T \underline{A}_{n+1} \underline{T}_1^T) \underline{S}_{n+1} = \begin{bmatrix} \lambda_1 & & & & & & & \\ & \lambda_2 & & & & & & \\ & & \ddots & & & & & \\ & & & \ddots & & & & \\ & & & & \ddots & & & \\ & & & & & \ddots & & \\ & & & & & & \lambda_{n+1} & \end{bmatrix} \quad (A.33)$$

$$\text{or } (\underline{T}_1 \underline{S}_{n+1})^T \underline{A}_{n+1} (\underline{T}_1 \underline{S}_{n+1}) = \underline{\Lambda} \quad (A.34)$$

$(\underline{T}_1 \underline{S}_{n+1})$ is the required orthogonal matrix and hence its $(n+1)$ columns are linearly independent. Clearly these are the eigenvectors of \underline{A}_{n+1} and hence the theorem is proved.

THEOREM 4. The derivations of the computational molecules using higher order correct monotone type approximations are presented here.

(a) Near the first boundary.

The finite difference expressions for the first and second order derivative can be obtained by expanding the function around that point using Taylor's series.

$$c_{i+1} = f(x+h) = f(x) + hf^I(x) + \frac{h^2}{2!} f^{II}(x) + \frac{h^3}{3!} f^{III}(x) + \frac{h^4}{4!} f^{IV}(x). \quad (A.35)$$

$$c_{i-1} = f(x-h) = f(x) - hf^I(x) + \frac{h^2}{2!} f^{II}(x) - \frac{h^3}{3!} f^{III}(x) + \frac{h^4}{4!} f^{IV}(x). \quad (A.36)$$

$f(x)$ refers to c_i .

The primes refer to the order of the derivatives.

Adding (A.35) and (A.36) gives

$$\begin{aligned} \therefore c_{i+1} + c_{i-1} &= 2c_i + h^2 \frac{\partial^2 c}{\partial z^2} + \frac{h^4}{2!} \frac{\partial^4 c}{\partial z^4} \\ \text{or } 12(c_{i+1} - 2c_i + c_{i-1}) &= 12h^2 \frac{\partial^2 c}{\partial z^2} + O|h^4|. \\ \text{or } \frac{\partial^2 c}{\partial z^2} &= \frac{1}{12h^2} \left[12c_{i+1} - 24c_i + 12c_{i-1} \right] \end{aligned} \quad (A.37)$$

Subtracting (A.36) from (A.35) gives

$$c_{i+1} - c_{i-1} = 2h f^I(x) + \frac{h^3}{3} f^{III}(x) \quad (A.37a)$$

$$\text{or } 3 h (c_{i+1} - c_{i-1}) = 6 h^2 \frac{\partial c}{\partial z} + O|h^4|.$$

$$\text{or } \frac{\partial c}{\partial z} = \frac{1}{12h^2} (6 h c_{i+1} - 6 h c_{i-1}) \quad (\text{A.38})$$

Hence the derivatives $\frac{\partial c}{\partial z}$ and $\frac{\partial^2 c}{\partial z^2}$ are replaced by (A.38)

and (A.37) respectively near the boundary to get the numerical solution.

(b) For all other points.

For this a five point molecule is considered and the expansion of these functions is considered $f(x + 2h)$, $f(x + h)$, $f(x - h)$, and $f(x - 2h)$.

The following are the identities.

$$\left. \begin{aligned} f(x + 2h) &\equiv c_{i+2} \\ f(x + h) &\equiv c_{i+1} \\ f(x) &\equiv c_i \\ f(x - h) &\equiv c_{i-1} \\ f(x - 2h) &\equiv c_{i-2} \end{aligned} \right\}$$

The expressions for $f(x + 2h)$, $f(x - 2h)$, $f(x + h)$ and $f(x - h)$ in terms of $f(x)$ and its derivatives are given by (A.40), (A.41), (A.35) and (A.36) $f(x + h)$ and $f(x - h)$ are given by (A.35) and (A.36).

$$\frac{3}{2} f(x + 2h) = \frac{3}{2} f(x) + 3hf^I(x) + 3h^2 f^{II}(x) + 2h^3 f^{III}(x) + O|h^4| \quad (A.40)$$

$$\frac{3}{2} f(x - 2h) = \frac{3}{2} f(x) - 3hf^I(x) + 3h^2 f^{II}(x) - 2h^3 f^{III}(x) + O|h^4| \quad (A.41)$$

Adding (A.40) and (A.41) and dividing by 2 gives

$$\frac{3}{4} f(x-2h) + \frac{3}{4} f(x + 2h) = \frac{3}{2} f(x) + 3h^2 f^{II}(x) + O|h^4| \quad (A.42)$$

$$\text{or } \frac{3}{4} c_{i+2} - \frac{3}{2} c_i + \frac{3}{4} c_{i-2} = 3h^2 \frac{\partial^2 c}{\partial z^2}$$

$$\text{or } 3h^2 \frac{\partial^2 c}{\partial z^2} = \frac{3}{4} c_{i+2} - \frac{3}{2} c_i + \frac{3}{4} c_{i-2} \quad (A.43)$$

Using equations (A.35) and (A.36) to get

$$12h^2 \frac{\partial^2 c}{\partial z^2} = 12 c_{i+1} - 24 c_i + 12 c_{i-1} \quad (A.44)$$

Subtracting (A.44) from (A.43) gives

$$-9h^2 \frac{\partial^2 c}{\partial z^2} = \frac{3}{4} c_{i+2} - 12 c_{i+1} + \frac{45}{2} c_i - 12 c_{i-1} + \frac{3}{4} c_{i-2}$$

$$\therefore -12h^2 \frac{\partial^2 c}{\partial z^2} = c_{i+2} - 16 c_{i+1} + 30 c_i - 16 c_{i-1} + c_{i-2} \quad (A.45)$$

$$\therefore \frac{\partial^2 c}{\partial z^2} = -\frac{1}{12h^2} \left[c_{i+2} - 16 c_{i+1} + 30 c_i - 16 c_{i-1} + c_{i-2} \right] \quad (A.46)$$

$$f(x + 2h) = f(x) + 2hf^I(x) + 2h^2f^{II}(x) + \frac{4}{3}h^3f^{III}(x) +$$

$$\frac{8}{12}h^4f^{IV}(x) \quad (A.47)$$

$$f(x - 2h) = f(x) - 2hf^I(x) + 2h^2f^{II}(x) - \frac{4}{3}h^3f^{III}(x) +$$

$$\frac{8}{12}h^4f^{IV}(x) \quad (A.48)$$

Subtracting (A.48) from (A.47)

$$f(x + 2h) - f(x - 2h) = 4hf^I(x) + \frac{8}{3}h^4f^{III}(x) \quad (A.49)$$

$$\text{or } hf(x + 2h) - hf(x - 2h) = 4h^2f^I(x) + \frac{8}{3}h^4f^{III}(x).$$

Multiplying throughout by $\frac{3}{8}$ gives

$$\frac{3}{8}hf(x + 2h) - \frac{3}{8}hf(x - 2h) = \frac{3}{2}h^2f^I(x) + O|h^4|$$

$$\text{or } \frac{3}{8}hc_{i+2} - \frac{3}{8}hc_{i-2} = \frac{3}{2}h^2 \frac{\partial c}{\partial z} \quad (A.50)$$

Using equation (A.37a) which is

$$c_{i+1} - c_{i-1} = 2hf^I(x) + \frac{h^3}{3}f^{III}(x)$$

$$\text{or } (hc_{i+1} - hc_{i-1}) = 2h^2 \left(\frac{\partial c}{\partial z} \right) + \frac{h^4}{3}f^{III}(x)$$

$$\text{or } 3hc_{i+1} - 3hc_{i-1} = 6h^2 \frac{\partial c}{\partial z} + O|h^4| \quad (A.51)$$

Equations (A.50) and (A.51) are

$$\frac{3}{2} h^2 \left(\frac{\partial c}{\partial z} \right) = \frac{3}{8} h c_{i+2} - \frac{3}{8} h c_{i-2} \quad (A.50)$$

$$6h^2 \left(\frac{\partial c}{\partial z} \right) = 3 h c_{i+1} - 3 h c_{i-1} \quad (A.51)$$

Subtracting (A.51) from (A.50) gives

$$-\frac{9}{2} h^2 \left(\frac{\partial c}{\partial z} \right) = \frac{3}{8} h c_{i+2} - 3 h c_{i+1} + 3 h c_{i-1} - \frac{3}{8} h c_{i-2}$$

$$\text{or } -12 h \left(\frac{\partial c}{\partial z} \right) = h c_{i+2} - 8 h c_{i+1} + 8 h c_{i-1} - h c_{i-2} \quad (A.52)$$

Hence

$$(A.53) \quad \frac{\partial c}{\partial z} = -\frac{1}{12h^2} \left[h c_{i+2} - 8 h c_{i+1} + 8 h c_{i-1} - h c_{i-2} \right]$$

Hence the derivatives $\frac{\partial c}{\partial z}$ and $\frac{\partial^2 c}{\partial z^2}$ are discretized

using equations (A.46) and (A.53) to get the semi analytical solution.

THEOREM 5. Any matrix $\underline{A}^{(n \times n)}$ is monotone if and only if there exists a real matrix $\underline{R}^{(n \times n)}$ with the following properties

$$\left. \begin{aligned} \underline{M} &= \underline{A} + \underline{R} \text{ is monotone} \\ \underline{M}^{-1} \underline{R} &\geq 0 \\ \rho(\underline{M}^{-1} \underline{R}) &< 1 \end{aligned} \right] \quad (A.54)$$

where ρ is the spectral radius of the matrix.

Proof: If \underline{A} is monotone, \underline{R} can be chosen to be the null matrix $\underline{0}$, and the above properties are trivially satisfied.

Now suppose \underline{A} is a real $(n \times n)$ matrix and \underline{R} is a real $(n \times n)$ matrix satisfying the set of properties represented by (A.54). Then

$$\underline{A} = \underline{M} - \underline{R} \quad (\text{A.55})$$

$$= \underline{M} (\underline{I} - \underline{M}^{-1} \underline{R}) \quad (\text{A.56})$$

$$\text{and } \underline{A}^{-1} = (\underline{I} - \underline{M}^{-1} \underline{R})^{-1} \underline{M}^{-1}$$

\therefore According to the theorem in Varga (29 p. 43) it can be easily shown that $\underline{M}^{-1} \underline{R}$ is convergent and \underline{A}^{-1} as in Varga (31) can be expressed as:

$$\underline{A}^{-1} = \left[\underline{I} + \underline{M}^{-1} \underline{R} + (\underline{M}^{-1} \underline{R})^2 + (\underline{M}^{-1} \underline{R})^3 + \dots \right] \underline{M}^{-1} \quad (\text{A.57})$$

As $\underline{M}^{-1} \underline{R}$ and \underline{M}^{-1} are both non-negative so it is clear from (A.57) that \underline{A}^{-1} is also non-negative.

Hence matrix \underline{A} is monotone.

INTRODUCTION TO APPENDICES B TO G

The various computer programs are listed in these appendices. A few important general aspects of the various programs are listed as given below.

1. The sample statement of each of the cases dealt with is given in the beginning of each program.
2. The programs are listed in the following general order
 - (a) a main line program, where normally the data are read in and the results are printed out.
 - (b) the calculations are performed in subroutines which in turn are called to the main line for the output of results.
3. The subroutines mainly used in this thesis are listed at the end in Appendix F. The subroutines which are specifically used in a certain problem are listed along with its main line program.
4. For a better understanding of various programs the "Comment Cards" have been added at various places.
5. In some of the programs exponent underflow occurred but this is not a serious problem. This does not affect the results to a great extent because the computer takes that number as zero and proceeds with the calculations. This is due to greater magnitude of the eigenvalues of the coefficient matrix.

APPENDIX B

ONE DIMENSIONAL HOMOGENEOUS CASE

The partial differential equation describing the above process is

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z}$$

$$0 \leq z \leq 1$$

The boundary conditions that have been used are:

(a) at $\theta = 0, c = 0$

at $z = 0, c = 1$

at $z = 1, \frac{\partial c}{\partial z} = 0.$

(b) at $\theta = 0, c = 0$

at $z = 0, c - \alpha \left(\frac{\partial c}{\partial z} \right)_{z \rightarrow 0^+} = c_{in}(\theta)$

at $z = 1, \frac{\partial c}{\partial z} = 0.$

Semi Analytical Solution A ten point and a twenty point grid are used for the given problem $0 \leq z \leq 1$. The grid spacing used is shown in Figure III-b.

Interpolated Values The results of ten point grid are derived from those of twenty point grid using interpolation.

Deviations (Errors)

= Interpolated value - value given by semi analytical solution.


```

C      SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C      DIMENSIONAL HOMOGENEOUS CASE
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
      REAL*8 DX
      DOUBLE PRECISION MATRIX(20,20),VECTOR(20,20)
      DOUBLE PRECISION X(20),VAR(20),CI(20),C1(20)
      DOUBLE PRECISION D(20,20),VICTOR(20,20)
      DOUBLE PRECISION CEVR(20,20),TIME(20),TOLERC
1,W(20,20)
C      READ THE DATA
      READ( 5,1) N,NT
      READ(5,5) ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 ) (X(J),J=1,N)
      READ( 5,2 ) (CI(J),J=1,N)
      READ( 5,2 ) (C1(J),J=1,N)
      READ(5,3) (TIME(J), J=1,NT)
      READ(5,4) DX
      NORM=2
      TOLERC=0.D00
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,220)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,223)
      WRITE(6,231)
      CALL LINECT(LINES,1,2)
      WRITE(6,232) (X(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,233)
      CALL LINECT(LINES,1,2)
      WRITE(6,234) (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,1,2)
      DO 30 J=1,N
30 C1(J)=C1(J)/(DX**2)

```



```

WRITE(6,234) (C1(J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,240)
DO 36 J=1,N
DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(DX**2)
36 CONTINUE
DO 31 J=1,N
CALL LINECT(LINES,1,2)
31 WRITE(6,241)(MATRIX(J,K),K=1,N)
CALL TRANS(N,DX,D,MATRIX)
LINES=9
WRITE(6,255)
CALL LINECT(LINES,1,2)
WRITE(6,241) (D(J,J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,259)
DO 50 J=1,N
CALL LINECT(LINES,1,2)
50 WRITE(6,241) (MATRIX(J,K),K=1,N)
CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NORM)
WRITE(6,220)
LINES =9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,242)
CALL LINECT(LINES,2,2)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,243)
DO 32 K=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
32 WRITE(6,223)
CALL CHECK(VECTOR,MATRIX,N,W)
CALL LINECT(LINES,1,2)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (W(J,K),K=1,N)
33 WRITE(6,223)
C CALCULATE THE TRANSPOSE OF THE MATRIX OF
C THE EIGENVECTORS
DO 40 I=1,N
DO 40 J=1,N
VICTOR(I,J)=VECTOR(J,I)
40 CONTINUE

```



```

C      A=(D(-1)*A(*)*D)
C      A(*)=THE ORIGINAL COEFFICIENT MATRIX
C      D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C      OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C      A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C      COEFFICIENT MATRIX A(*)
C      Q=THE MATRIX OF EIGENVECTORS OF A
C      CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C      COEFFICIENT MATRIX
      DO 38 I=1,N
      DO 38 J=1,N
      VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,3,2)
      WRITE(6,223)
      WRITE(6,256)
      CALL LINECT(LINES,2,2)
      WRITE(6,232) (MATRIX(J,J),J=1,N)
      CALL LINECT(LINES,3,2)
      WRITE(6,223)
      WRITE(6,257)
      DO 39 K=1,N
      CALL LINECT(LINES,3,2)
      WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
C      (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
C      QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
C      D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
C      CALCULATE THE PRODUCT (QT*D(-1))
      DO 41 I=1,N
      DO 41 J=1,N
      VICTOR(I,J)=VICTOR(I,J)/D(J,J)
41 CONTINUE
      CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
1CEVR,VICTOR)
      WRITE(6,220)
      WRITE(6,225)
      WRITE(6,245)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,248)
      DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,249)
      DO 35 J=1,NT
35 WRITE(6,251) TIME(J), (CEVR(J,K),K=6,10 )

```


C

FORMAT STATEMENTS

```

1  FORMAT(1X,2I4)
2  FORMAT(10F8.5)
3  FORMAT(11F7.3)
4  FORMAT(1X,F16.8)
5  FORMAT(10F8.5)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
      111HDIMENSIONAL/25X,22H   HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,19HUSING ORDINARY B.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX)
241 FORMAT(1H,10X,10F5.1)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
      12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
      18X,2H 9, 8X, 2H10)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
255 FORMAT(1H,10X,9HMATRIX(D)/10X,
      119H(DIAGONAL ELEMENTS))
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
      127HORIGINAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
      127HORIGINAL COEFFICIENT MATRIX)
259 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX/
      120X,26H(CONVERTED INTO SYMMETRIC))
      STOP
      END

```


CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

INITIAL CONDITION VECTOR

CONDITION VECTOR				
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

BOUNDARY CONDITION VECTOR				
27.2990	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

ORIGINAL COEFFICIENT MATRIX

[illegible]

MATRIX(D)

(DIAGONAL ELEMENTS)

-1.0 1.3 -1.6 2.1 -2.6 3.4 -4.3 5.5 -7.0 8.9

ORIGINAL COEFFICIENT MATRIX

(CONVERTED INTO SYMMETRIC)

[illegible]

EIGENVALUES

2.362764	85.752492	60.055819	35.156755	6.334014
79.575516	70.989428	13.507177	47.748475	23.397493

EIGENVECTORS

0.089301	0.127548	-0.403341	0.423819	-0.193317
-0.243816	0.338529	-0.300001	0.432589	0.378072

-0.174016	0.243893	-0.300533	-0.176935	0.349676
-0.403866	0.425041	0.428492	0.073726	-0.365414

0.249791	0.338813	0.179412	-0.349952	-0.418237
-0.425163	0.195132	-0.312014	-0.420024	-0.024892

-0.312736	0.403972	0.434214	0.323033	0.387766
-0.300390	-0.180042	0.017157	-0.145311	0.389472

0.359617	0.433645	0.144125	0.215093	-0.265479
-0.072415	-0.421184	0.287508	0.395259	-0.351541

-0.388026	0.425227	-0.326826	-0.412829	0.080330
0.180439	-0.348777	-0.427805	0.212675	-0.049701

0.396503	0.379456	-0.387645	-0.042745	0.123840
0.371301	-0.016724	0.323526	-0.359013	0.399578

-0.384614	0.300353	0.037988	0.430675	-0.298687
0.434599	0.327779	-0.034287	-0.273861	-0.336499

0.352969	0.194867	0.415951	-0.137052	0.402809
0.348584	0.428268	-0.274554	0.312338	-0.074345

-0.303192	0.072263	0.271940	-0.373458	-0.411552
0.142810	0.209934	0.426432	0.327093	0.408355

CHECK OF SIMILARITY TRANSFORMATION

44.098236	21.417811	0.000000	-0.000000	0.000000
0.000000	-0.000000	0.000000	0.000000	0.000000

21.417811	44.098236	21.417811	0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	0.000000

0.000000	21.417811	44.098236	21.417811	0.000000
----------	-----------	-----------	-----------	----------

0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	21.417811	44.098236	21.417811
0.000000	-0.000000	0.000000	0.000000	0.000000

..CONTD

0.000000	-0.000000	0.000000	21.417811	44.098236
21.417811	0.000000	0.000000	-0.000000	0.000000

0.000000	-0.000000	0.000000	0.000000	21.417811
44.098236	21.417811	0.000000	-0.000000	-0.000000

-0.000000	0.000000	0.000000	-0.000000	0.000000
21.417811	44.098236	21.417811	-0.000000	-0.000000

0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	21.417811	44.098236	21.417811	-0.000000

0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	-0.000000	21.417811	44.098236	21.417811

0.000000	0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	21.417811	27.296808

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

2.362764	85.052492	60.056819	35.156755	6.334014
79.575516	70.989428	13.507177	47.748475	23.397493

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.080301	-0.127548	0.403341	-0.423819	0.198317
0.243816	-0.338529	0.300001	-0.432589	-0.378072

-0.221828	0.310905	-0.383108	-0.225550	0.445754
-0.514832	0.541825	0.546225	0.093983	-0.465815

-0.405915	-0.550577	-0.291547	0.568678	0.679642
0.690897	-0.317093	0.507027	0.682546	0.040450

-0.647836	0.836831	0.899478	0.669165	0.803261
-0.622261	-0.372958	0.035541	-0.301013	0.806795

-0.949633	-1.145118	-0.380587	-0.567990	0.701043
0.191225	1.112212	-0.759216	-1.043751	0.928307

-1.306187	1.431413	-1.100173	-1.389681	0.270408
0.607401	-1.174066	-1.440092	0.715914	-0.167305

-1.701454	-1.628301	1.663442	0.183426	-0.531417
-1.593309	0.071765	-1.333297	1.540575	-1.714647

-2.103911	1.642988	0.207803	2.355871	-1.633871
2.377336	1.793015	-0.187556	-1.498073	-1.840713

-2.461314	-1.358843	-2.900499	0.955691	-2.808858
-2.430743	-2.986394	1.914514	-2.177992	0.518420

-2.695121	0.642360	2.417312	-3.319723	-3.658345
1.269457	1.866134	3.790617	2.907579	3.629925

SOLUTION OF THE DISPERSION MODELEQUATION
 USING ORDINARY B.C.
 SEMI-ANALYTICAL SOLUTION

TIME	CONCENTRATIONS AT GRID POINTS				
	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.760229	0.510666	0.291627	0.144062	0.062142
0.2	0.881334	0.726742	0.556463	0.393956	0.257437
0.3	0.926401	0.825387	0.703163	0.570308	0.439040
0.4	0.950320	0.880261	0.791245	0.687702	0.576317
0.5	0.964788	0.914290	0.848156	0.767982	0.677198
0.6	0.974247	0.936889	0.886949	0.824733	0.751912
0.7	0.980764	0.952630	0.914467	0.866020	0.808051
0.8	0.985428	0.963985	0.934579	0.896753	0.850804
0.9	0.988861	0.972391	0.949613	0.920028	0.883711
1.0	0.991440	0.978734	0.961036	0.937880	0.909239

TIME	CONCENTRATIONS AT GRID POINTS				
	6	7	8	9	10
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.023652	0.008024	0.002449	0.000681	0.000194
0.2	0.155309	0.085648	0.044886	0.021995	0.011623
0.3	0.320244	0.221320	0.145574	0.093349	0.064813
0.4	0.464881	0.361055	0.271609	0.202702	0.161786
0.5	0.580801	0.484962	0.396816	0.324837	0.280299
0.6	0.671641	0.588621	0.509292	0.442366	0.400025
0.7	0.742582	0.673173	0.605290	0.546912	0.509507
0.8	0.798071	0.741264	0.684892	0.635839	0.604167
0.9	0.841577	0.795707	0.749758	0.709477	0.683343
1.0	0.875757	0.839047	0.802044	0.769446	0.748232

GUIDE POINTS

INITIAL CONDITION VECTOR

BOUNDARY CONDITION VECTOR

ORIGINAL COEFFICIENT MATRIX

25.7-16.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-27.3	44.1-16.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0-27.3	44.1-16.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0-27.3	44.1-16.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0-27.3	44.1-16.8	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0-27.3	44.1-16.8	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0-27.3	44.1-16.8	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0-27.3	44.1-16.8	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0-27.3	44.1-16.8	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0-27.3	27.3	27.3

MATRIX (U)

(DIAGONAL ELEMENTS)

-1.0 1.3 -1.6 2.1 -2.6 3.4 -4.3 5.5 -7.0 8.9

ORIGINAL COEFFICIENT MATRIX

(CONVERTED INTO SYMMETRIC)

[illegible]

EIGENVALUES

1.354825	34.673754	4.690060	57.993504	51.925487
78.910611	12.842532	69.615175	44.917610	20.193424

EIGENVECTORS

0.235535	0.274123	-0.404508	-0.277393	0.378232
-0.146282	0.426444	0.210655	0.332596	0.411477

-0.317231	0.224847	0.396244	-0.417535	0.110571
-0.363657	-0.225122	0.442510	0.299972	-0.105123

0.339935	0.315934	-0.324471	0.308263	-0.441072
-0.444806	0.031907	0.310174	-0.321159	-0.294147

-0.353001	0.396621	0.200774	0.422861	0.140091
-0.359328	0.245742	-0.070958	-0.311257	0.423426

0.356060	0.432386	-0.044947	0.264391	0.361455
-0.139243	-0.413374	-0.394715	0.309251	-0.187607

-0.349024	0.439462	-0.118073	-0.252601	-0.345503
0.133003	0.346108	-0.399320	0.323086	-0.221802

0.332024	0.308131	0.262198	-0.427055	-0.165101
0.355425	-0.301367	-0.081949	-0.206891	0.437164

-0.305749	0.318185	-0.364364	-0.222760	0.432336
0.444713	-0.042475	0.302756	-0.334446	-0.266125

0.270728	0.227384	0.406221	0.412381	-0.084575
0.367393	0.318506	0.441763	0.284096	-0.140137

-0.228048	0.071150	-0.286752	0.286574	-0.391271
0.152454	-0.430204	0.225576	0.345314	0.422535

CHECK OF SIMILARITY TRANSFORMATION

25.665171	21.417811	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	0.000000	-0.000000

21.417811	44.998466	21.417811	0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	0.000000

-0.000000	21.417811	44.998466	21.417811	-0.000000
-----------	-----------	-----------	-----------	-----------

0.000000 -0.000000 -0.000000 -0.000000 0.000000

-0.000000 0.000000 21.417811 44.098236 21.417811
0.000000 -0.000000 0.000000 0.000000 0.0

..CONTD

-0.000000 -0.000000 -0.000000 21.417811 44.098236
21.417811 0.000000 0.000000 -0.000000 0.000000

0.000000 -0.000000 -0.000000 0.000000 21.417811
44.098236 21.417811 -0.000000 -0.000000 -0.000000

-0.000000 0.000000 -0.000000 -0.000000 0.000000
21.417811 44.098236 21.417811 0.000000 -0.000000

-0.000000 -0.000000 -0.000000 0.000000 0.000000
-0.000000 21.417811 44.098236 21.417811 -0.000000

0.000000 -0.000000 -0.000000 0.000000 -0.000000
-0.000000 0.000000 21.417811 44.098236 21.417811

-0.000000 0.000000 -0.000000 -0.000000 0.000000
-0.000000 -0.000000 -0.000000 21.417811 27.296808

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

1.869805	4.017756	4.699962	57.303524	31.926287
72.910611	10.842333	62.615175	+4.917612	20.143424

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.285525	-0.074045	0.404608	0.277393	-0.378232
0.146290	-0.426444	-0.214665	-0.332596	-0.411477

-0.404304	0.261132	0.505117	-0.532257	0.140952
-0.463576	-0.378219	0.501545	0.381116	-0.134006

-0.552333	-0.512398	0.527271	-0.013427	0.716746
0.722818	-0.051687	-0.504237	0.521884	0.477984

-0.731244	0.421749	0.415904	0.375960	0.290200
-0.744351	0.589057	-0.145990	-0.544771	0.847845

-0.940238	-1.160225	0.118690	-0.647933	-0.954487
0.357697	1.041587	1.042317	-0.816633	0.500692

-1.174997	1.430470	-0.397462	-0.849977	-1.183061
0.447719	1.332224	-1.344205	1.287580	-0.746637

-1.425784	-1.708446	-1.125129	1.332555	0.708474
-1.525122	0.865180	0.347762	1.274002	-1.275935

-1.672506	1.750906	-1.903127	-0.124533	2.403250
2.432610	-0.453980	1.556121	-1.829481	-1.455755

-1.887892	-1.449212	-2.845500	-2.875606	0.589760
-2.561895	-2.904672	-3.080492	-1.981054	0.977200

-2.627151	0.806608	-3.437893	2.555174	-3.473067
1.355188	-2.124148	1.997393	3.069540	3.759971

SOLUTION OF THE DISPERSION MODEL EQUATION
 USING HANDEWATS S.C.
 SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.432038	0.257611	0.137594	0.064475	0.026672
0.2	0.591735	0.453387	0.327305	0.218943	0.136079
0.3	0.694182	0.585614	0.473060	0.364758	0.267816
0.4	0.768657	0.677073	0.532353	0.484574	0.389275
0.5	0.812575	0.744129	0.585417	0.580499	0.493210
0.6	0.850748	0.794688	0.629574	0.657151	0.579990
0.7	0.879117	0.833631	0.679830	0.718670	0.651857
0.8	0.901171	0.864114	0.719685	0.768352	0.711239
0.9	0.918559	0.888278	0.751588	0.808680	0.760298
1.0	0.932423	0.907626	0.777333	0.841574	0.800851

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.006817	0.003241	0.000968	0.000254	0.000074
0.2	0.073568	0.042182	0.021127	0.010043	0.005165
0.3	0.186970	0.124109	0.078639	0.048681	0.032810
0.4	0.391511	0.225254	0.163247	0.117572	0.091231
0.5	0.407766	0.323418	0.259385	0.205337	0.172772
0.6	0.501368	0.425191	0.356112	0.300053	0.265432
0.7	0.581875	0.512134	0.447184	0.393289	0.359502
0.8	0.652255	0.588305	0.529575	0.480131	0.443839
0.9	0.707920	0.653962	0.602224	0.558222	0.530198
1.0	0.753315	0.710006	0.665186	0.626825	0.602286


```

C   SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C   DIMENSIONAL HOMOGENEOUS CASE
C       INPUT DATA
C   N= THE NUMBER OF GRID POINTS.
C   NT = THE TOTAL NO. OF TIMES.
C   MATRIX=THE COEFFICIENT MATRIX
C   X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C   CI= THE INITIAL CONDITION VECTOR.
C   C1= THE BOUNDARY CONDITION VECTOR.
C   TIME= THE DIMENSIONLESS TIMES.
C   DX= THE GRID SPACING.
      REAL*8 DX
      DOUBLE PRECISION MATRIX(40,40),VECTOR(40,40),
1TOLERC,W(40,40),CEVR(40,40),TIME(40)
      DOUBLE PRECISION X(40),VAR(40),CI(40),C1(40)
      DOUBLE PRECISION D(40,40),VICTOR(40,40)
C       READ THE DATA
      READ( 5,1)  N,NT
      READ(5,5)  ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 )  (X(J),J=1,N)
      READ( 5,2 )  (CI(J),J=1,N)
      READ( 5,2 )  (C1(J),J=1,N)
      READ(5,3)  (TIME(J), J=1,NT)
      READ(5,4) DX
      NORM=2
      TOLERC=0.D00
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,220)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,223)
      WRITE(6,231)
      CALL LINECT(LINES,1,2)
      WRITE(6,232) (X(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,233)
      CALL LINECT(LINES,2,2)
      WRITE(6,234) (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,2,2)
      DO 30 J=1,N
30  C1(J)=C1(J)/(DX**2)
      WRITE(6,234) (C1(J),J=1,N)

```



```

DO 36 J=1,N
DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(DX**2)
36 CONTINUE
WRITE(6,220)
WRITE(6,240)
CALL LINECT(LINES,4,2)
DO 31 J=1,N
WRITE(6,241) (MATRIX(J,K),K=1,N)
31 CONTINUE
CALL TRANS(N,DX,D,MATRIX)
LINES=9
WRITE(6,255)
CALL LINECT(LINES,1,2)
WRITE(6,241) (D(J,J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,220)
WRITE(6,261)
DO 50 J=1,N
CALL LINECT(LINES,1,2)
50 WRITE(6,241) (MATRIX(J,K),K=1,N)
CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NORM)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,6,2)
WRITE(6,242)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,243)
DO 32 K=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
32 WRITE(6,223)
CALL CHECK(VECTOR,MATRIX,N,W)
CALL LINECT(LINES,1,2)
WRITE(6,223)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232) (W(J,K),K=1,N)
33 WRITE(6,223)
CALCULATE THE TRANSPOSE OF THE MATRIX OF
THE EIGENVECTORS
DO 40 I=1,N
DO 40 J=1,N
VECTOR(I,J)=VECTOR(J,I)
40 CONTINUE
A=(D(-1)*A(*)*D)
A(*)=THE ORIGINAL COEFFICIENT MATRIX

```



```

C      D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C      OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C      A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C      COEFFICIENT MATRIX A(*)
C      Q=THE MATRIX OF EIGENVECTORS OF A
C      CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C      COEFFICIENT MATRIX
      DO 38 I=1,N
      DO 38 J=1,N
      VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,6,2)
      WRITE(6,256)
      WRITE(6,232) (MATRIX(J,J),J=1,N)
      CALL LINECT(LINES,3,2)
      WRITE(6,223)
      WRITE(6,257)
      DO 39 K=1,N
      CALL LINECT(LINES,7,2)
      WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
      (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
      QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
      D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
      CALCULATE THE PRODUCT (QT*D'1)
      DO 41 I=1,N
      DO 41 J=1,N
      VICTOR(I,J)=VICTOR(I,J)/D(J,J)
41 CONTINUE
      CALL SEMIAN(N,VAR,VECTOR,C1,CI,MATRIX,TIME,NT,
1CEVR,VICTOR)
      WRITE(6,220)
      WRITE(6,225)
      WRITE(6,245)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,248)
      DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,249)
      DO 35 J=1,NT
35 WRITE(6,251) TIME(J), (CEVR(J,K),K=6,10 )
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,259)
      DO 45 J=1,NT

```



```

45 WRITE(6,251) TIME(J), (CEVR(J,K),K=11,15)
   WRITE(6,223)
   WRITE(6,246)
   WRITE(6,260)
   DO 46 J=1,NT

```

```

46 WRITE(6,251) TIME(J), (CEVR(J,K),K=16,20)
      FORMAT STATEMENTS

```

```

1  FORMAT(1X,2I4)
2  FORMAT(10F8.5)
3  FORMAT(11F7.3)
4  FORMAT(1X,F16.8)
5  FORMAT(10F8.5)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
      111HDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,19HUSING ORDINARY B.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,19H COEFFICIENT MATRIX)
241 FORMAT(1H,10F6.1)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
      12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
      18X,2H 9, 8X, 2H10)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
255 FORMAT(1H,10X,9HMATRIX(D)/10X,
      119H(DIAGONAL ELEMENTS))
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
      127HORIGINAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
      127HORIGINAL COEFFICIENT MATRIX)
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,
      18X,2H14,8X,2H15)
260 FORMAT(1H,15X,5H TIME,9X,2H16,8X,2H17,8X,2H18,
      18X,2H19,8X,2H20)
261 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX/
      120X,26H(CONVERTED INTO SYMMETRIC))

```


B-21

STOP
END

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.040780	0.007350	0.146340	0.105120	0.243900
0.202680	0.341460	0.390240	0.439020	0.487800
0.535980	0.585360	0.634140	0.682920	0.731700
0.780430	0.829260	0.878040	0.926820	0.975600

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

04.3060	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

(CONVERTED INTO SYMMETRIC)

EIGENVALUES

2.368924	332.842042	202.264345	149.522285	6.527054
327.130395	474.656495	25.594940	100.551707	224.826498
248.065151	78.177077	14.273089	317.670488	288.453447
40.255135	57.920492	259.441120	174.970839	124.520621

EIGENVECTORS

0.032914	0.047572	-0.306105	0.309887	-0.075009
-0.094033	0.179311	-0.160857	-0.234802	-0.203415
-0.273861	0.262255	0.118852	0.138291	0.216134
-0.199447	-0.233337	-0.247808	-0.311638	-0.300899
-0.065384	0.094035	-0.118034	-0.069025	0.145286
-0.179327	0.223522	0.274797	0.230700	-0.190514
-0.262509	-0.232711	-0.210170	0.247948	0.311819
0.305064	0.308461	-0.301146	-0.025655	0.157205
0.096973	0.133202	0.260592	-0.294512	-0.206396
-0.247957	0.301168	-0.308597	0.038075	0.157750
0.022233	0.042507	0.285310	0.306268	0.233729
-0.269014	-0.173887	-0.117932	0.309525	0.218766
-0.127294	0.179331	0.218518	0.134628	0.254486
-0.293544	0.193473	0.252373	-0.310120	0.306781
0.282820	0.236882	-0.306456	0.301175	0.025384
0.105618	-0.078787	0.157882	0.051137	-0.271500
0.155820	0.216172	-0.175331	0.264525	-0.286520
-0.311852	0.025358	-0.122550	0.193054	0.050852
0.049823	-0.247472	0.280724	0.203724	-0.197107
0.105614	0.277991	0.309727	-0.305316	-0.076921
-0.182284	0.247461	-0.286511	-0.193546	0.302478
-0.301180	-0.157304	-0.043017	0.186174	-0.272202
-0.044352	0.084218	-0.210733	0.117679	-0.309752
-0.263479	-0.289337	0.213373	-0.078272	0.311687

..CONTD

0.206291	0.273756	0.265853	-0.221414	-0.295479
-0.262518	-0.233430	0.196037	-0.373819	-0.235943
-0.292337	0.227285	0.107869	-0.222372	-0.249774
0.305852	0.152842	-0.044449	0.299037	-0.085921

-0.227516	0.293549	0.311904	0.242864	0.271838
-0.199463	-0.306822	-0.291880	0.059848	0.111767
-0.235867	-0.307456	0.011817	-0.157991	-0.050599
-0.200264	0.152435	-0.272369	0.100892	-0.266798

0.245674	0.306281	0.054417	0.167318	-0.231047
-0.117870	-0.218315	0.302591	0.255355	0.311942
0.066248	0.124352	-0.129659	-0.260898	0.176774
0.001068	-0.304232	-0.286424	-0.290731	0.225310

-0.260519	0.311456	-0.290321	-0.280133	0.175680
-0.025324	-0.050547	-0.225045	-0.266630	0.100345
0.299368	0.173404	0.227283	-0.309786	0.305633
0.198627	0.240402	-0.075578	-0.124824	0.149084

0.271852	0.310143	-0.166596	-0.104920	-0.109229
0.069575	0.135572	0.081863	-0.039444	-0.243710
0.220711	-0.311282	-0.289462	-0.294532	0.264105
-0.305480	-0.025185	0.194612	0.280455	-0.303199

-0.279520	0.301182	0.226682	0.303504	0.035888
0.153000	0.272471	0.085197	0.293570	-0.266061
-0.087805	0.162157	0.306501	-0.218298	0.075480
0.263546	-0.216137	0.311992	0.147913	0.009323

0.283418	0.295183	0.254004	0.037317	0.030710
0.211759	0.310448	-0.227408	-0.202333	0.062795
-0.304877	0.136476	-0.275743	-0.096862	-0.155270
-0.107621	0.310665	0.184394	-0.268278	0.298328

-0.283496	0.262019	-0.123738	-0.311816	-0.112819
0.293972	0.045714	0.303291	-0.134725	0.308760
-0.204434	-0.309270	0.201984	0.044628	-0.289489
-0.104699	-0.104107	-0.087991	-0.169499	-0.165186

..CONTD

0.273741	-0.233721	-0.303645	0.032137	0.178801
0.303745	0.075403	-0.290715	0.311431	0.147154
0.103917	-0.196221	-0.096726	0.176878	-0.270805
0.267041	-0.054165	-0.291285	0.264283	-0.212027

-0.272234	0.199460	0.011652	0.304657	-0.233503
0.306830	-0.112284	0.193346	-0.117466	-0.208700
0.308836	0.096222	-0.023616	0.272504	-0.092860
-0.306033	0.265730	-0.265861	0.190932	0.275459

0.261047	0.140538	0.308138	-0.099927	0.273474
0.275350	-0.259205	-0.039585	-0.216309	-0.289064
0.187118	-0.301434	0.140274	0.211704	0.132737
0.201079	-0.236830	-0.031632	-0.238505	0.067851

-0.246340	0.117865	0.107165	-0.232384	-0.290192
0.218283	-0.312021	-0.125722	0.292629	0.012144
-0.129475	0.228207	-0.235058	0.286375	0.241300
-0.002137	0.126322	0.227374	-0.210572	-0.311409

0.228311	0.072437	-0.266816	0.162896	0.300222
-0.140931	-0.251555	0.254360	-0.020657	0.297321
-0.311226	0.065692	0.293186	0.201740	0.287610
-0.197805	0.109081	0.307895	0.221230	0.094845

-0.207205	0.026316	-0.210049	0.246100	-0.285313
0.050482	-0.009760	-0.308809	-0.275901	0.190027
-0.168851	-0.208043	-0.305542	0.075346	0.123578
0.305286	-0.208004	0.145655	0.226785	0.261857

CHECK OF SIMILARITY TRANSFORMATION

168.103362	83.419890	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000

83.419890	168.103362	83.419890	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	0.000000	0.000000	0.000000

..CONTD

-0.000000	83.419590	168.103362	83.419590	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000

-0.000000	-0.000000	83.419590	168.103362	83.419590
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000

0.000000	-0.000000	-0.000000	83.419590	168.103362
83.419590	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

0.000000	0.000000	-0.000000	-0.000000	83.419590
168.103362	83.419590	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000

0.000000	0.000000	0.000000	-0.000000	-0.000000
83.419590	168.103362	83.419590	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	83.419590	168.103362	83.419590	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000

-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	83.419590	168.103362	83.419590
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000

-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	83.419590	168.103362
83.419590	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000

..CONTD

-0.000000	-0.000000	0.0	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	83.419590
168.103362	83.419590	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000

0.000000	-0.000000	0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
83.419590	168.103362	83.419590	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000

0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	83.419590	168.103362	83.419590	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	0.000000

-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	83.419590	168.103362	83.419590
-0.000000	-0.000000	0.000000	0.000000	0.000000

0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	83.419590	168.103362
83.419590	-0.000000	-0.000000	-0.000000	0.000000

0.000000	0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	83.419590
168.103362	83.419590	-0.000000	-0.000000	-0.000000

0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
83.419590	168.103362	83.419590	-0.000000	-0.000000

0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	83.419590	168.103362	83.419590	-0.000000

..CONTD

0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	83.419590	188.103362	83.419590

-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	83.419590	84.205986

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

2.308924	332.093032	200.260885	142.522285	6.527054
227.190395	304.656495	25.594940	100.551707	224.826495
243.055131	76.177077	14.273089	317.670493	233.453447
40.256135	57.920653	369.441120	174.970830	124.520621

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.032914	-0.047573	0.306105	-0.309887	0.075009
0.094032	-0.179111	0.160857	0.234892	0.293415
0.273861	-0.262255	-0.113852	-0.155291	-0.215134
0.199447	0.233537	0.247898	0.311638	0.300890

-0.072910	0.106296	-0.133424	-0.078025	0.164229
-0.202729	0.331794	0.310626	0.250731	-0.225529
-0.296737	-0.319572	-0.247747	0.280278	0.352476
0.345523	0.348480	-0.342411	-0.029001	0.177703

-0.123910	-0.176715	-0.332977	0.376320	0.263728
0.316833	-0.334025	0.394305	-0.125313	-0.201569
-0.028400	-0.354114	-0.354561	-0.391342	-0.299053
0.343730	0.222180	0.150691	-0.395504	-0.279534

-0.183803	0.259122	0.315623	0.194450	0.367574
-0.423098	0.238115	0.364523	-0.447931	0.443108
0.409944	0.342156	-0.443361	0.435011	-0.035664
0.153997	-0.112709	0.223042	0.073861	-0.392149

-0.254452	-0.352946	0.287898	-0.431892	0.467803
0.509183	-0.041401	0.200089	-0.249893	-0.083027
-0.407807	0.436339	-0.458357	-0.381602	0.321319
-0.172436	-0.053313	-0.505643	0.498492	0.125500

-0.336422	0.857636	-0.523763	-0.357227	0.594553
-0.555855	-0.291537	-0.079301	0.343611	-0.502374
-0.081950	0.165132	-0.383977	0.217557	-0.571678
-0.495501	-0.572152	0.403927	-0.140757	0.575240

..CONTD

-0.430371	-0.571536	-0.137344	0.461022	0.616437
0.547676	-0.592758	-0.408979	0.633837	0.492232
0.609884	-0.432328	-0.225040	0.046672	0.521088
-0.638079	-0.214857	0.092730	-0.623861	0.179251

-0.536548	0.602461	0.735548	0.572735	0.641062
-0.470382	-0.723564	-0.688326	0.141136	0.263575
-0.556232	-0.725054	0.027866	-0.372581	-0.119326
-0.472273	0.859470	-0.642314	0.257924	-0.629176

-0.654022	-0.816465	-0.145061	-0.446026	0.615911
0.314211	0.581971	-0.806627	-0.680710	-0.831554
-0.175598	-0.231490	0.345638	0.695484	-0.471234
-0.002848	0.911001	0.763530	0.775012	-0.600017

-0.785027	0.000722	-0.376635	-0.344129	0.520379
-0.075310	-0.152815	-0.678134	-0.803439	0.302370
0.972090	0.522521	0.684874	-0.333481	0.920968
0.598524	0.751527	-0.227729	-0.376135	0.449237

-0.925936	-1.055412	0.567460	0.357331	0.372058
-0.236997	-0.461787	-0.278842	0.134353	0.830127
-0.751789	1.060201	-0.985968	1.003239	-0.890801
1.040528	0.389737	-0.662890	-0.055289	1.032761

-1.076245	1.159654	0.872300	1.168590	0.133179
0.608327	1.040106	0.323038	1.149596	-1.024424
-0.338090	0.624760	1.180132	-0.840514	0.290621
1.037841	-0.832700	1.201273	0.569513	0.035897

-1.238561	-1.241222	-1.105519	-0.162419	-0.172069
-1.008700	-1.351184	0.989763	0.880624	-0.273308
1.326932	-0.503904	1.200135	0.421578	0.675792
0.458474	-1.152125	-0.802550	1.167645	-1.298435

-1.394760	1.201556	-0.633372	-1.534089	-0.855052
1.397102	1.159631	1.492151	-0.662626	1.519057
-1.009788	-1.521609	0.993752	0.217563	-1.473442
-0.914659	-0.055420	-0.432303	-0.836364	-0.812690

..CONTINUED

-1.555791	-1.249221	1.633675	-0.179725	-0.904376
-1.722878	-0.419447	1.516764	-1.731974	-0.818372
-2.675724	-1.095174	0.537927	-0.983677	1.534406
-1.497115	0.301225	1.619926	-1.414157	1.174155

-1.711332	1.258221	0.773253	1.415222	-1.467513
1.928875	-0.725367	1.215463	-0.733449	-1.311964
1.941422	0.672742	-0.148458	1.713092	-0.627764
-1.923877	1.672552	-1.671326	1.200232	1.724811

-1.855235	-1.142229	-2.182676	0.710595	-1.943347
-1.956682	1.341252	0.291292	1.537121	2.254130
-1.329568	2.142383	-0.796810	-2.215052	-0.242245
-1.428898	2.107315	0.225134	1.595275	-0.422162

-1.978771	0.246772	0.360827	-2.268202	-2.370215
1.752400	-2.595365	-1.009889	2.350601	2.097547
-1.042030	1.031512	-1.833150	2.300362	2.340402
-0.017143	1.014702	1.826426	-1.591461	-2.501450

-2.073273	-0.657731	2.422699	-1.479105	-2.726035
-1.279657	2.234122	-2.309603	0.167567	-2.692693
2.825947	-0.575682	-2.662141	-1.531864	-2.611515
1.796076	-1.130235	-2.795649	-2.008775	-0.861195

-2.126741	0.259645	-2.155940	2.525963	-2.926440
0.513141	-1.223935	-3.164611	-2.831845	1.950432
-1.733078	-2.955462	-3.136590	0.773347	1.268399
3.133468	-2.053703	1.576263	2.348234	2.687690

SOLUTION OF THE DISPERSION MODEL EQUATION
USING ORDINARY D.C.
SERI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	-0.000000	-0.000000
0.1	0.001806	0.766533	0.633223	0.501429	0.380020
0.2	0.045107	0.873021	0.803465	0.720811	0.533974
0.3	0.063947	0.924306	0.875690	0.820497	0.759792
0.4	0.076906	0.943515	0.914841	0.875079	0.832225
0.5	0.083532	0.963129	0.938794	0.910412	0.878007
0.6	0.087802	0.972691	0.954571	0.933299	0.908797
0.7	0.090759	0.979286	0.965501	0.949250	0.930443
0.8	0.092872	0.984010	0.973358	0.960731	0.946169
0.9	0.094429	0.987491	0.979160	0.969321	0.957874
1.0	0.095597	0.990138	0.983521	0.975770	0.966740

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.0	0.000000	-0.000000	0.000000	0.000000	0.000000
0.1	0.275327	0.190566	0.125973	0.079536	0.047977
0.2	0.543127	0.460396	0.379566	0.305856	0.240785
0.3	0.684898	0.627198	0.558435	0.490214	0.424088
0.4	0.784055	0.732176	0.677280	0.620525	0.562938
0.5	0.841727	0.801844	0.756756	0.712979	0.665138
0.6	0.881065	0.850190	0.816345	0.779819	0.740979
0.7	0.909002	0.884935	0.858312	0.829280	0.798075
0.8	0.920447	0.910581	0.889589	0.865552	0.841620
0.9	0.924744	0.920857	0.913299	0.895023	0.875160
1.0	0.926374	0.924629	0.921491	0.916984	0.901179

CONCENTRATIONS AT GRID POINTS

TIME	11	12	13	14	15
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	0.027664	0.015258	0.008056	0.004075	0.001977
0.2	0.135129	0.138977	0.101852	0.072858	0.050902
0.3	0.302435	0.303386	0.260785	0.204181	0.163856
0.4	0.505378	0.443995	0.304800	0.345742	0.296709
0.5	0.616953	0.565226	0.515834	0.468726	0.422927
0.6	0.700313	0.558412	0.615984	0.573860	0.533014
0.7	0.765000	0.730582	0.695292	0.659854	0.625119
0.8	0.815020	0.737108	0.758259	0.720169	0.700430
0.9	0.853882	0.821441	0.808184	0.784567	0.761176
1.0	0.884255	0.866254	0.847601	0.828612	0.809759

CONCENTRATIONS AT GRID POINTS

TIME	16	17	18	19	20
0.0	-0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.000422	0.000412	0.000173	0.000076	0.000037
0.2	0.004752	0.023261	0.015424	0.010492	0.008014
0.3	0.129641	0.102207	0.080793	0.065789	0.057658
0.4	0.293555	0.213154	0.183409	0.166619	0.154502
0.5	0.333571	0.342936	0.311517	0.289123	0.275001

0.6	0.459914	0.438507	0.418467	0.398133
0.7	0.522716	0.502261	0.481784	0.460624
0.8	0.572363	0.547842	0.520363	0.490647
0.9	0.718740	0.718157	0.700514	0.667116
1.0	0.741637	0.774980	0.750583	0.743637

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

DATA POINTS

0.044780	0.00755	0.141340	0.195120	0.243900
0.292650	0.341450	0.390240	0.439020	0.487800
0.536580	0.585360	0.634140	0.682920	0.731700
0.730430	0.820260	0.873040	0.926820	0.975600

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

18.4872	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

COEFFICIENT MATRIX

APPENDIX (C)

(DIAGONAL ELEMENTS)

(CONVERTED INTO SYMMETRIC)

EIGENVALUES

1.317389	332.390649	4.772234	194.967018	143.253098
325.821267	34.734771	316.857764	117.729937	222.285823
11.069145	256.542043	93.671326	313.252378	21.101735
280.342185	51.658716	244.341350	169.008770	71.465899

EIGENVECTORS

0.180237	0.225336	-0.272697	-0.213973	0.252138
-0.051630	0.307113	0.077241	-0.265791	-0.193754
0.302254	-0.149757	0.279606	-0.101969	-0.309012
0.126257	-0.302746	0.172298	-0.232615	-0.291368

-0.105348	0.074681	0.285205	-0.263265	0.152084
-0.145132	-0.212042	0.207358	-0.280927	-0.297193
-0.294435	-0.212735	0.204423	-0.257823	0.263855
0.202530	0.146631	0.313969	-0.214070	0.072877

0.208930	0.121538	-0.287652	0.129194	-0.295813
-0.224504	0.031303	0.292720	0.314659	0.007847
0.252009	-0.212294	-0.283615	-0.315732	-0.155951
0.233945	0.006365	0.114644	0.230493	0.206944

-0.220875	0.165613	0.276979	0.304369	-0.063243
-0.282019	0.161052	0.314620	-0.109082	0.302102
-0.179962	0.053057	0.248566	-0.253593	0.010962
0.117331	-0.280727	-0.209195	0.216502	-0.312611

0.231090	0.205634	-0.254635	-0.031017	0.314806
-0.312079	-0.289378	0.263309	-0.248789	0.181131
0.086763	0.232466	0.061830	-0.095288	0.136634
-0.123641	0.205793	-0.305330	-0.228143	0.155201

-0.239497	0.240421	0.221562	-0.314857	-0.031302
-0.211757	0.201507	0.163829	0.259315	-0.183797
0.016634	0.279057	-0.303724	0.099322	-0.251733
-0.292500	-0.132175	-0.070308	-0.218978	0.132819

..CONT'D

0.248027	0.269421	-0.170153	-0.370377	-0.305408
-0.281083	-0.192405	0.223331	0.292200	-0.290231
-0.118076	0.247339	0.209180	0.255200	0.305977
-0.291062	-0.111297	0.241574	0.225765	-0.309065

-0.252632	0.291323	0.122194	0.292194	0.123024
-0.223045	0.006654	-0.121335	-0.314990	0.001615
0.205640	-0.224024	0.117091	0.315751	-0.284216
-0.113970	0.287534	0.291087	0.221429	0.225217

0.253274	0.307070	-0.073792	0.164472	0.268453
-0.143292	0.132167	-0.240194	0.098009	0.300242
-0.263033	-0.311759	-0.313655	0.255352	0.202678
0.121016	-0.290067	0.024455	-0.223363	0.045162

-0.253932	0.314813	0.015281	-0.232229	-0.203649
-0.049590	-0.207337	-0.305379	0.255307	0.186198
0.302804	-0.143352	0.162772	0.007947	-0.067942
0.291498	0.117363	-0.268737	-0.223853	-0.201010

0.252602	0.314332	0.043375	-0.241511	-0.207296
0.049841	0.204101	-0.307211	-0.252473	-0.183767
-0.297223	0.141089	0.163421	-0.096665	-0.082951
0.292153	0.126235	-0.270058	0.220933	0.277375

-0.243295	0.307154	-0.101181	0.161455	0.265906
0.142707	-0.172302	-0.240839	-0.103345	-0.301152
0.253701	0.311421	-0.313047	-0.254557	0.214117
0.122500	-0.293578	0.021927	0.226251	-0.040315

0.244035	0.201347	0.154224	0.293505	0.127437
0.222590	-0.018529	-0.122253	0.314885	-0.004617
-0.180775	0.225000	0.113399	-0.315745	-0.204366
-0.113321	0.283557	0.290097	-0.218473	-0.230672

-0.236864	0.269591	-0.200769	-0.066938	-0.304179
0.237783	0.297035	0.022338	-0.086799	0.298264
0.093543	-0.045113	0.214096	-0.256985	0.304613
-0.292323	-0.102251	0.243157	-0.228622	0.307537

..CONTD

-0.227839	0.240541	0.233854	-0.315069	-0.036083
0.311651	-0.304467	0.152978	-0.262471	0.191194
0.004271	-0.278377	-0.301329	-0.100599	-0.242422
-0.293221	-0.140037	-0.067835	0.215996	-0.125594

-0.217329	0.205781	-0.265874	-0.034522	0.315016
0.312179	0.284576	0.267783	0.245294	-0.178665
-0.106584	-0.283394	0.055323	0.094204	0.122582
-0.125218	0.298843	-0.305193	-0.230965	-0.162042

0.204520	0.155891	0.283650	0.303943	-0.058525
0.282314	-0.150569	0.314533	0.114349	-0.302956
0.106369	-0.056334	0.252584	0.252895	0.026409
0.115727	-0.276314	-0.211086	-0.213480	0.313312

-0.190410	0.121937	-0.298473	0.132401	-0.297440
0.224965	-0.043790	0.293092	-0.314344	-0.010847
-0.263073	0.217772	-0.280674	0.315714	-0.169120
0.289263	0.036861	0.112279	-0.233284	-0.200914

0.174908	0.074798	0.281141	-0.261306	0.147854
0.145715	0.220670	0.208108	0.075470	0.296171
0.293856	0.313216	-0.002150	0.253597	0.271613
0.294265	0.155066	0.313599	0.210957	-0.080563

-0.157838	0.026221	-0.261962	-0.216540	0.253035
0.052278	-0.309025	0.073006	0.268771	0.198114
-0.207512	0.151603	0.282592	0.103242	-0.309515
0.127827	-0.303316	0.174416	0.235573	0.294243

CHECK OF SIMILARITY TRANSFORMATION

92.320772	83.419590	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000

83.419590	168.173362	83.419590	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000

..CONTI

-0.000000	83.419590	168.103362	83.419590	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	83.419590	168.103362	83.419590
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	83.419590	168.103362
83.419590	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	83.419590
168.103362	83.419590	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
83.419590	168.103362	83.419590	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	83.419590	168.103362	83.419590	-0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	83.419590	168.103362	83.419590
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
83.419590	-0.000000	-0.000000	83.419590	168.103362
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000

..CONT0

0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	83.419590
168.103362	83.419590	-0.000000	-0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
83.419590	168.103362	83.419590	-0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	83.419590	168.103362	83.419590	-0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	83.419590	168.103362	83.419590	83.419590
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
83.419590	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	83.419590
168.103362	83.419590	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
83.419590	168.103362	83.419590	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	83.419590	168.103362	83.419590	-0.000000

..CONT

0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	83.419590	168.173362	83.419590

-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	83.419590	94.325986

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

1.917389	332.302648	4.779204	194.267218	143.050098
426.821267	34.734771	316.857364	117.729937	220.285823
11.062145	266.542148	92.671326	303.252372	21.101735
266.242185	51.658215	244.341856	169.703770	71.465899

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.130227	-0.005096	0.272647	0.213973	-0.250138
0.051630	-0.307113	-0.077041	0.265791	-0.193754
-0.302254	0.149750	-0.273606	0.101969	0.309012
-0.126257	0.390746	-0.172298	0.232815	0.291368

-0.220819	0.084418	0.323522	-0.297591	0.171914
-0.164055	-0.284590	0.224395	-0.091478	-0.335944
-0.332826	-0.353511	0.005079	-0.291430	0.293256
0.331925	0.165750	0.354907	-0.241903	0.082379

-0.266965	-0.155423	0.367555	-0.165081	0.377982
0.285365	-0.040753	-0.374030	-0.402063	-0.010026
-0.322011	0.260208	0.362347	0.403435	0.190270
-0.370486	-0.122750	-0.145489	-0.294518	-0.264423

-0.319027	0.239208	0.400063	0.440347	-0.091347
-0.407343	0.232629	0.454430	-0.157556	0.436350
-0.259934	0.077934	0.359023	-0.366438	0.015833
0.169471	-0.405477	-0.302156	0.312711	-0.451530

-0.377303	-0.345576	0.415745	0.250642	-0.513987
0.503534	0.472470	-0.433071	0.466199	-0.295734
-0.141659	-0.462000	-0.100950	0.155578	-0.223084
0.261870	-0.482953	0.499331	0.372491	-0.253397

-0.442013	0.643719	0.408913	-0.581098	-0.057771
-0.575375	0.596625	0.302362	0.478589	-0.348442
0.039700	0.516987	-0.560569	0.183307	-0.484606
-0.539984	-0.249063	-0.129760	-0.404144	0.245130

..CONT'D

-0.513271	-0.862075	0.373754	0.146822	0.637147
0.586495	0.402236	-0.049716	-0.192351	0.624266
0.248334	-0.090885	-0.436393	-0.534493	-0.640426
0.607222	0.232193	-0.533980	-0.471001	0.644782

-0.531053	0.408131	0.304672	0.623067	0.290121
-0.525996	0.015632	-0.286137	-0.742826	0.003809
0.484950	-0.526505	0.276130	0.744620	-0.632044
-0.282919	0.678375	0.585455	0.522184	0.531119

-0.675160	-0.818589	0.196710	-0.438439	-0.715638
0.381980	-0.485600	0.640294	-0.261265	-0.800365
0.717170	0.831063	-0.836123	-0.580700	-0.540286
-0.322597	0.773243	-0.865190	0.595426	-0.123386

-0.765177	0.948631	0.046046	-0.720872	-0.613659
-0.143429	-0.897456	-0.925025	0.770827	0.561074
0.905418	-0.433519	0.490482	0.295146	-0.204731
0.878376	0.353667	-0.809789	-0.674530	-0.846772

-0.860416	-1.072407	-0.140446	0.322637	0.706095
-0.166703	-1.001760	1.046425	0.359997	0.625947
1.012394	-0.463639	-0.573677	0.329266	0.282547
-0.095135	-0.429982	0.919873	-0.752545	-0.944797

-0.950967	1.182046	-0.389581	0.621656	1.023829
0.540469	-0.563422	-0.927311	-0.397916	-1.159537
0.996066	1.109074	-1.205336	-0.980131	0.824424
0.472047	-1.138372	0.084425	0.871141	-0.155225

-1.062129	-1.270650	-0.671241	-1.277440	-0.554653
-0.960748	0.081000	0.532089	-1.370437	0.020094
0.825977	-0.981482	-0.482673	1.374239	1.281190
0.515230	-1.234187	-1.262610	0.950895	1.003071

-1.165837	1.328250	-0.997755	-0.329320	-1.486520
1.381414	0.096237	0.112361	-0.427041	1.467418
0.484818	-0.222432	1.053324	-1.264329	1.498655
-1.423691	-0.503057	1.195497	-1.124789	1.513040

..CONTD

-1.247048	-1.338241	-1.223349	1.752167	0.290672
-1.733201	1.693237	-0.906375	1.459691	-1.063293
-0.223755	1.551395	1.679130	0.550464	1.348192
1.620702	0.763242	0.377255	-1.201229	0.598473

-1.364246	1.203038	-1.677698	-0.217019	1.982341
1.962502	1.760394	1.683413	1.542035	-1.123170
-0.670036	-1.704597	0.347659	0.500951	0.772606
-0.727181	1.376662	-1.918588	1.451964	-1.018675

-1.453248	-1.175842	-2.015655	-2.159867	0.415386
-2.006166	1.070673	-2.235119	-2.812578	2.152848
-1.305424	0.292182	-1.704900	-1.707102	-0.187667
-0.822442	1.263631	1.500005	1.517087	-2.226444

-1.522501	0.973484	-2.317213	1.063534	-2.332241
1.807076	-0.251754	2.354318	-2.525031	-0.087131
-2.113181	1.740294	-2.254567	2.536037	-1.358487
2.323563	0.677729	0.901399	-1.873896	-1.613885

-1.587267	-0.680082	-2.552772	2.372676	-1.342526
-1.323096	-2.003772	-1.889631	-0.635272	-2.680244
-2.713624	-2.062192	0.012522	-2.348072	-2.466259
-2.671939	-1.408007	-2.848401	-1.915504	0.731516

-1.620044	0.259136	-2.688774	-2.222656	2.557142
0.536581	-3.171420	0.800650	2.758660	2.012910
-3.074160	1.956050	2.900518	1.059076	-3.175857
1.312014	-3.112226	1.790129	2.417913	3.020099

SOLUTION OF THE DISPERSION MODEL EQUATION
USING DANKOWITZ'S D.C.
SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.405346	0.407153	0.317463	0.232504	0.167016
0.2	0.657666	0.582349	0.510954	0.439853	0.371536
0.3	0.765220	0.691751	0.635359	0.577040	0.517940
0.4	0.825343	0.764521	0.720024	0.672364	0.623658
0.5	0.848616	0.815143	0.780704	0.742542	0.701981
0.6	0.873992	0.854144	0.825672	0.794672	0.761303
0.7	0.893634	0.882852	0.859307	0.834516	0.807044
0.8	0.921807	0.904964	0.886195	0.865479	0.842826
0.9	0.935499	0.922255	0.906889	0.889860	0.871152
1.0	0.947216	0.935939	0.923503	0.909260	0.893782

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.115137	0.076116	0.048234	0.029294	0.017052
0.2	0.307701	0.249691	0.198415	0.154323	0.117434
0.3	0.489203	0.401947	0.347201	0.295349	0.248590
0.4	0.673098	0.521932	0.470025	0.420832	0.372366
0.5	0.657421	0.615327	0.570215	0.524640	0.479177
0.6	0.725783	0.683392	0.649466	0.609393	0.568609
0.7	0.777502	0.745054	0.712913	0.678350	0.642689
0.8	0.813291	0.791960	0.763970	0.734512	0.703826
0.9	0.850779	0.828789	0.805279	0.780355	0.754228
1.0	0.875363	0.853526	0.830827	0.817663	0.795775

CONCENTRATIONS AT GRID POINTS

TIME	11	12	13	14	15
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.009516	0.005093	0.002616	0.001290	0.000611
0.2	0.087402	0.063605	0.045252	0.031471	0.021393
0.3	0.205215	0.168109	0.135252	0.107246	0.083864
0.4	0.328173	0.282813	0.242753	0.206454	0.173942
0.5	0.434410	0.390921	0.349284	0.310064	0.273835
0.6	0.527594	0.485869	0.447002	0.408608	0.372314
0.7	0.605314	0.563671	0.533276	0.497728	0.463724
0.8	0.672210	0.641065	0.607618	0.576026	0.545346
0.9	0.727133	0.699380	0.671362	0.643564	0.616580
1.0	0.772758	0.749271	0.725347	0.701197	0.677775

CONCENTRATIONS AT GRID POINTS

TIME	16	17	18	19	20
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.000274	0.000122	0.000052	0.000022	0.000010
0.2	0.017235	0.009292	0.004013	0.002901	0.002491
0.3	0.054307	0.044727	0.038341	0.030504	0.026323
0.4	0.105703	0.121999	0.113064	0.089441	0.081053
0.5	0.141207	0.212359	0.139617	0.172540	0.163038

0.6	0.33078	0.309620	0.235102	0.260081	0.255570
0.7	0.430045	0.413701	0.380028	0.361248	0.352243
0.8	0.546571	0.492661	0.463776	0.452332	0.443055
0.9	0.591117	0.563122	0.546011	0.533911	0.525604
1.0	0.655695	0.635002	0.618037	0.605735	0.598515


```

C          PROGRAM  FOR INTERPOLATION
C  INTERPOLATE THE VALUES OF CONCENTRATION
C  CORRESPONDING TO ONE GRID FROM THOSE
C  OF A HIGHER POINT GRID
C  N= THE NUMBER OF GRID POINTS ( THE VALUES
C  TO BE INTERPOLATED)
C  NN= THE NUMBER OF GRID POINTS ( GREATER THAN
C  ABOVE)
C  NT= THE TOTAL NUMBER OF TIMES
C  X= THE DIMENSIONLESS DISTANCES OF THE GRID
C  POINTS CORRESPONDING TO THE VALUES TO BE
C  INTERPOLATED)
C  XX= THE DIMENSIONLESS DISTANCES OF THE GRID
C  POINTS (CORRESPONDING TO THE HIGHER POINT GRID)
REAL X(10),XX(30),TIME(15),CONC(15,10),
1CEVR(15,20),CGRID(15,10)
REAL CINTP(15,10),ERROR(15,10)
INTEGER I,J,N,NN,NT
READ(5,1)  N,NN,NT
READ(5,2)  (TIME(J),J=1,NT)
DO 3 J=1,NT
READ(5,6)  (CEVR(J,K),K=1,NN)
3 CONTINUE
DO 5 J=1,NT
READ(5,6)  (CONC(J,K),K=1,N)
5 CONTINUE
READ(5,13)  (X(J),J=1,N)
READ(5,13)  (XX(J),J=1,NN)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,4,2)
WRITE(6,261)
CALL LINECT(LINES,3,2)
WRITE(6,262) (X(I),I=1,N)
WRITE(6,222)
WRITE(6,263)
CALL LINECT(LINES,3,2)
WRITE(6,262) (XX(I),I=1,NN)
WRITE(6,223)
WRITE(6,225)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,247)
WRITE(6,248)
DO 7 J=1,NT
7 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)

```



```

WRITE(6,246)
WRITE(6,249)
DO 8 J=1,NT
8 WRITE(6,251) TIME(J),(CEVR(J,K),K=6,10)
WRITE(6,220)
WRITE(6,246)
WRITE(6,259)
DO 15 J=1,NT
15 WRITE(6,251) TIME(J),(CEVR(J,K),K=11,15)
WRITE(6,223)
WRITE(6,246)
WRITE(6,258)
DO 16 J=1,NT
16 WRITE(6,251) TIME(J),(CEVR(J,K),K=16,20)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,3,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,250)
WRITE(6,248)
DO 9 J=1,NT
9 WRITE(6,251) TIME(J),(CONC(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)
WRITE(6,249)
DO 17 J=1,NT
17 WRITE(6,251) TIME(J),(CONC(J,K),K=6,10)
CALL CALCU(20,N,NT,CEVR,1,X,TIME,CINTP,XX)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,260)
WRITE(6,248)
DO 10 J=1,NT
10 WRITE(6,251) TIME(J),(CINTP(J,K),K=1,5)
WRITE(6,223)
WRITE(6,249)
DO 30 J=1,NT
30 WRITE(6,251) TIME(J),(CINTP(J,K),K=6,10)
DO 27 J=1,NT
DO 27 K=1,N
27 ERROR(J,K)=CINTP(J,K)-CONC(J,K)
WRITE(6,220)
WRITE(6,255)
WRITE(6,223)
WRITE(6,248)
DO 11 J=1,NT
11 WRITE(6,251) TIME(J),(ERROR(J,K),K=1,5)

```



```
WRITE(6,223)
```

```
WRITE(6,255)
```

```
WRITE(6,223)
```

```
WRITE(6,249)
```

```
DO 29 J=1,NT
```

```
29 WRITE(6,251) TIME(J), (ERROR(J,K),K=6,10)
```

```
FORMAT STATEMENTS
```

```
1 FORMAT(1X,3I3)
```

```
2 FORMAT(10F7.3)
```

```
6 FORMAT(5F16.6)
```

```
13 FORMAT(10F8.5)
```

```
220 FORMAT(1H2)
```

```
222 FORMAT(1H,//)
```

```
223 FORMAT(1H,/)
```

```
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,  
18HEQUATION/20X,19HUSING ORDINARY B.C.)
```

```
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
```

```
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
```

```
247 FORMAT(1H,40X,17HTWENTY POINT GRID)
```

```
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,  
12H 3, 8X, 2H 4, 8X, 2H 5)
```

```
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,  
18X,2H 9, 8X, 2H10)
```

```
250 FORMAT(1H,40X,14HTEN POINT GRID)
```

```
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
```

```
255 FORMAT(1H,30X,18H ASSOCIATED ERRORS)
```

```
258 FORMAT(1H,15X,5H TIME,9X,2H16,8X,2H17,8X,2H18,  
18X,2H19,8X,2H20)
```

```
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,  
18X,2H14,8X,2H15)
```

```
260 FORMAT(1H,30X,20H INTERPOLATED VALUES)
```

```
261 FORMAT(1H,25X,27HGRID POINTS(TEN POINT GRID))
```

```
262 FORMAT(1H,10X,5F10.6)
```

```
263 FORMAT(1H,25X,30HGRID POINTS(TWENTY POINT GRID))
```

```
STOP
```

```
END
```


GRID PLINTS(TEN POINT GRID)

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

GRID PLINTS(TWENTY POINT GRID)

0.048780	0.097560	0.146340	0.195120	0.243900
0.292680	0.341460	0.390240	0.439020	0.487800
0.536580	0.585360	0.634140	0.682920	0.731700
0.780480	0.829260	0.878040	0.926820	0.975600

SOLUTION OF THE DISPERSION MODELEQUATION USING ORDINARY D.C.

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS TWENTY POINT GRID

TIME	1	2	3	4	5
0.1	0.891896	0.766633	0.633223	0.501429	0.380020
0.2	0.945107	0.879021	0.803465	0.720811	0.633974
0.3	0.965947	0.924386	0.875690	0.820497	0.759792
0.4	0.976906	0.948515	0.914841	0.875979	0.832225
0.5	0.983502	0.963129	0.938794	0.910412	0.878007
0.6	0.987802	0.972691	0.954571	0.933299	0.908797
0.7	0.990759	0.979286	0.965501	0.949256	0.930443
0.8	0.992873	0.984010	0.973358	0.960781	0.946169
0.9	0.994429	0.987491	0.979160	0.969321	0.957874
1.0	0.995597	0.990108	0.983531	0.975770	0.966740

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	0.212327	0.190566	0.125973	0.079536	0.047977
0.2	0.346127	0.460396	0.379566	0.305856	0.240785
0.3	0.574856	0.627198	0.558435	0.490214	0.424088
0.4	0.764086	0.732176	0.677380	0.620625	0.562938
0.5	0.841727	0.801844	0.758756	0.712979	0.665138
0.6	0.881065	0.850190	0.816349	0.779819	0.740979
0.7	0.905062	0.884935	0.858312	0.829230	0.798075
0.8	0.925447	0.910581	0.889589	0.866552	0.841620
0.9	0.944744	0.929887	0.913299	0.895023	0.875160
1.0	0.958374	0.944629	0.931491	0.916984	0.901179

TIME	CONCENTRATIONS AT GRID POINTS				
	11	12	13	14	15
0.1	0.027604	0.015250	0.008050	0.004075	0.001977
0.2	0.135129	0.138977	0.101852	0.072868	0.050902
0.3	0.301455	0.303386	0.250785	0.204181	0.165856
0.4	0.505370	0.448995	0.394800	0.343742	0.296709
0.5	0.615953	0.566220	0.516834	0.468726	0.422927
0.6	0.700313	0.658412	0.615984	0.573860	0.533014
0.7	0.765030	0.730582	0.695292	0.659854	0.625119
0.8	0.815028	0.787100	0.758299	0.729169	0.700430
0.9	0.855002	0.831441	0.808184	0.784567	0.761176
1.0	0.884202	0.866254	0.847601	0.828612	0.809759

TIME	CONCENTRATIONS AT GRID POINTS				
	16	17	18	19	20
0.1	0.000921	0.000412	0.000178	0.000076	0.000037
0.2	0.034752	0.023261	0.015429	0.010492	0.008014
0.3	0.129801	0.102207	0.080793	0.065769	0.057658
0.4	0.254555	0.218154	0.188459	0.160819	0.154802
0.5	0.380571	0.342936	0.311517	0.288123	0.275001
0.6	0.494584	0.459914	0.430602	0.408567	0.390133
0.7	0.592114	0.562001	0.536509	0.517184	0.506244
0.8	0.672903	0.647842	0.626363	0.610081	0.600047
0.9	0.738740	0.718157	0.700514	0.687110	0.679510
1.0	0.791637	0.774980	0.760683	0.749013	0.743637

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS
TEN POINT GRID

TIME	1	2	3	4	5
0.1	0.709229	0.510666	0.291627	0.144062	0.062142
0.2	0.681334	0.726742	0.556463	0.393956	0.257437
0.3	0.926401	0.625587	0.703163	0.570308	0.439040
0.4	0.950320	0.880261	0.791245	0.687702	0.576317
0.5	0.964788	0.914290	0.848156	0.767982	0.677198
0.6	0.974247	0.936869	0.885949	0.824733	0.751912
0.7	0.980764	0.952630	0.914467	0.866020	0.808051
0.8	0.985428	0.963985	0.934579	0.896753	0.850804
0.9	0.988861	0.972391	0.949613	0.920028	0.883711
1.0	0.991440	0.976734	0.961036	0.937880	0.909239

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	0.023652	0.008024	0.002449	0.000681	0.000194
0.2	0.155309	0.086648	0.044886	0.021995	0.011623
0.3	0.323244	0.221320	0.145574	0.093349	0.064813
0.4	0.464861	0.361055	0.271609	0.202702	0.161786
0.5	0.580801	0.484962	0.396816	0.324637	0.280299
0.6	0.671641	0.588621	0.509292	0.442366	0.400025
0.7	0.742562	0.673173	0.605290	0.546912	0.509507
0.8	0.798071	0.741264	0.684892	0.635839	0.604167
0.9	0.841577	0.795707	0.749758	0.709477	0.683343
1.0	0.875757	0.839047	0.802044	0.769446	0.748232

INTERPOLATED VALUES					
TIME	1	2	3	4	5
0.1	0.772774	0.513056	0.289120	0.136001	0.054327
0.2	0.882373	0.728899	0.558604	0.394462	0.255434
0.3	0.926524	0.825999	0.704324	0.571525	0.439549
0.4	0.949984	0.879890	0.791180	0.687984	0.576684
0.5	0.964187	0.913285	0.847129	0.767175	0.676663
0.6	0.973477	0.935460	0.885215	0.823002	0.750398
0.7	0.979883	0.950909	0.912221	0.863566	0.805674
0.8	0.984471	0.962063	0.931962	0.893742	0.847707
0.9	0.987852	0.970324	0.946721	0.916536	0.880017
1.0	0.990352	0.976561	0.957936	0.934096	0.905047

TIME	6	7	8	9	10
0.1	0.018149	0.005125	0.001231	0.000254	0.000043
0.2	0.151206	0.081683	0.040285	0.018383	0.008886
0.3	0.315432	0.215013	0.142062	0.089184	0.060654
0.4	0.464905	0.360337	0.269965	0.200262	0.159317
0.5	0.580420	0.484536	0.396199	0.324088	0.279961
0.6	0.670453	0.587790	0.508835	0.442370	0.400849
0.7	0.740522	0.671616	0.604388	0.546794	0.510401
0.8	0.795185	0.738858	0.683195	0.635011	0.604360
0.9	0.837943	0.792433	0.747106	0.707622	0.682405
1.0	0.871460	0.834941	0.798398	0.766445	0.745989

ASSOCIATED ERRORS

TIME	1	2	3	4	5
C.1	0.003545	0.002990	-0.002507	-0.007261	-0.007815
C.2	0.001044	0.002157	0.002141	0.000536	-0.002093
C.3	0.000123	0.003612	0.001161	0.001217	0.000509
C.4	-0.000336	-0.000371	-0.000064	0.000282	0.000367
C.5	-0.000601	-0.001005	-0.001027	-0.000806	-0.000535
C.6	-0.000770	-0.001429	-0.001734	-0.001731	-0.001514
C.7	-0.000881	-0.001720	-0.002240	-0.002454	-0.002377
C.8	-0.000957	-0.001922	-0.002617	-0.003011	-0.003097
C.9	-0.001009	-0.002067	-0.002892	-0.003442	-0.003694
1.0	-0.001048	-0.002173	-0.003100	-0.003784	-0.004192

ASSOCIATED ERRORS

TIME	6	7	8	9	10
C.1	-0.003503	-0.002895	-0.001218	-0.000427	-0.000140
C.2	-0.004103	-0.004965	-0.004601	-0.003612	-0.002737
C.3	-0.000812	-0.002307	-0.003512	-0.004165	-0.004159
C.4	0.000024	-0.000718	-0.001646	-0.002440	-0.002469
C.5	-0.000381	-0.000426	-0.000617	-0.000749	-0.000338
C.6	-0.001188	-0.000831	-0.000457	0.000004	0.000824
C.7	-0.002080	-0.001557	-0.000902	-0.000118	0.000894
C.8	-0.002866	-0.002406	-0.001697	-0.000828	0.000193
C.9	-0.003634	-0.003274	-0.002652	-0.001855	-0.000938
1.0	-0.004297	-0.004106	-0.003646	-0.003001	-0.002243


```

C          PROGRAM FOR INTERPOLATION
C  INTERPOLATE THE VALUES OF CONCENTRATION
C  CORRESPONDING TO ONE GRID FROM THOSE
C  OF A HIGHER POINT GRID
C  N= THE NUMBER OF GRID POINTS ( THE VALUES
C  TO BE INTERPOLATED)
C  NN= THE NUMBER OF GRID POINTS ( GREATER THAN
C  ABOVE)
C  NT= THE TOTAL NUMBER OF TIMES
C  GRIDX=THE DIMENSIONLESS DISTANCES OF GRID POINTS
C  (CORRESPONDING TO THE VALUES TO BE INTERPOLATED)
C  GRIDN=THE DIMENSIONLESS DISTANCES OF GRID POINTS
C  (CORRESPONDING TO THE HIGHER POINT GRID)
REAL GRIDX(10),GRIDN(20),TIME(15),CONC(15,10)
1,CEVR(15,20),WORK(300)
REAL CINTP(15,10),ERROR(15,10),X,F(300),ARG(20)
1,Z(20),Y,YY(20),VAL(300)
INTEGER I,J,N,NN,NT
READ(5,1) N,NN,NT
READ(5,2) (TIME(J),J=1,NT)
DO 3 J=1,NT
READ(5,6) (CEVR(J,K),K=1,NN)
3 CONTINUE
DO 5 J=1,NT
READ(5,6) (CONC(J,K),K=1,N)
5 CONTINUE
READ(5,13) (GRIDX(J),J=1,N)
READ(5,13) (GRIDN(J),J=1,NN)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,4,2)
WRITE(6,264)
CALL LINECT(LINES,3,2)
WRITE(6,265) (GRIDX(I),I=1,N)
WRITE(6,222)
WRITE(6,266)
CALL LINECT(LINES,3,2)
WRITE(6,265) (GRIDN(I),I=1,NN)
WRITE(6,223)
WRITE(6,225)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,245)
WRITE(6,247)
WRITE(6,248)
DO 7 J=1,NT
7 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)

```



```

WRITE(6,246)
WRITE(6,249)
DO 8 J=1,NT
8 WRITE(6,251) TIME(J), (CEVR(J,K),K=6,10)
WRITE(6,220)
WRITE(6,246)
WRITE(6,259)
DO 15 J=1,NT
15 WRITE(6,251) TIME(J), (CEVR(J,K),K=11,15)
WRITE(6,223)
WRITE(6,246)
WRITE(6,258)
DO 16 J=1,NT
16 WRITE(6,251) TIME(J), (CEVR(J,K),K=16,20)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,3,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,250)
WRITE(6,248)
DO 9 J=1,NT
9 WRITE(6,251) TIME(J), (CONC(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)
WRITE(6,249)
DO 17 J=1,NT
17 WRITE(6,251) TIME(J), (CONC(J,K),K=6,10)
DO 14 JJ=1,NN
Z(JJ)=GRIDN(JJ)
14 CONTINUE

```

THE TABLE OF Z VS F READY FOR ONE VALUE OF TIME

ORDER THE TABLE USING S.S.P

```

IROW=20
ICUL=1
NDIM=20
DO 19 J=1,NT
DO 19 I=1,N
X=GRIDX(I)
DO 31 JJ=1,NN
F(JJ)=CEVR(J,JJ)
31 CONTINUE
CALL ATSG(X,Z,F,WORK,IROW,ICUL,ARG,VAL,NDIM)
EPS=2.00001
CALL ALI(X,ARG,VAL,Y,NDIM,EPS,IER)

```



```

      YY(I)=Y
      CINTP(J,I)=YY(I)
19  CONTINUE
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,260)
      WRITE(6,248)
      DO 20 J=1,NT
20  WRITE(6,251)  TIME(J),(CINTP(J,K),K=1,5)
      WRITE(6,223)
      WRITE(6,249)
      DO 30 J=1,NT
30  WRITE(6,251)  TIME(J), (CINTP(J,K),K=6,10)
      DO 27 J=1,NT
      DO 27 K=1,N
27  ERROR(J,K)=CINTP(J,K)-CONC(J,K)
      WRITE(6,223)
      WRITE(6,255)
      WRITE(6,223)
      WRITE(6,248)
      DO 23 J=1,NT
28  WRITE(6,251)  TIME(J), (ERROR(J,K),K=1,5)
      WRITE(6,223)
      WRITE(6,255)
      WRITE(6,223)
      WRITE(6,249)
      DO 29 J=1,NT
29  WRITE(6,251)  TIME(J), (ERROR(J,K),K=6,10)

```

FORMAT STATEMENTS

```

1  FORMAT(1X,3I3)
2  FORMAT(10F7.3)
6  FORMAT(5F16.6)
13 FORMAT(10F8.5)
220 FORMAT(1H2)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,21HUSING DANCKWERTS B.C.)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
247 FORMAT(1H,40X,17HTWENTY POINT GRID)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
      12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME, 9X, 2H 6, 8X, 2H 7, 8X, 2H 8,
      18X, 2H 9, 8X, 2H 10)
250 FORMAT(1H,40X,14HTEN POINT GRID)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
255 FORMAT(1H,30X,18H ASSOCIATED ERRORS)
258 FORMAT(1H,15X,5H TIME, 9X, 2H 16, 8X, 2H 17, 8X, 2H 18,

```



```
18X,2H19,8X,2H20)  
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,  
18X,2H14,8X,2H15)  
260 FORMAT(1H,30X,20H INTERPOLATED VALUES)  
264 FOPMAT(1H,25X,27HGRID POINTS(TEN PCINT GRID))  
265 FORMAT(1H,10X,5F10.6)  
266 FORMAT(1H,25X,30HGRID POINTS(TWENTY POINT GRID))  
STOP  
END
```


GRID POINTS(TEN POINT GRID)

C.095240	C.190480	C.285720	C.380960	C.476200
C.571440	C.666680	C.761920	C.857160	C.952400

GRID POINTS(TWENTY POINT GRID)

C.048780	C.097560	C.146340	C.195120	C.243900
C.292680	C.341460	C.390240	C.439020	C.487800
C.536580	C.585360	C.634140	C.682920	C.731700
C.780480	C.829260	C.878040	C.926820	C.975600

SOLUTION OF THE DISPERSION MODEQUATION
USING LANCHEWITS B.C.

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS
TWENTY POINT GRID

TIME	1	2	3	4	5
0.1	C.496396	C.400163	C.310963	C.232504	C.167016
0.2	C.653666	C.582899	C.510954	C.439853	C.371536
0.3	C.745220	C.691751	C.635550	C.577040	C.517940
0.4	C.805843	C.764521	C.720024	C.672864	C.623658
0.5	C.848616	C.816143	C.780704	C.742542	C.701981
0.6	C.879992	C.854144	C.825672	C.794672	C.761303
0.7	C.905634	C.882852	C.859607	C.834516	C.807044
0.8	C.921809	C.904964	C.886195	C.865479	C.842828
0.9	C.935959	C.922255	C.906889	C.889860	C.871152
1.0	C.947216	C.935939	C.923303	C.909260	C.893782

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	C.115137	C.076116	C.046234	C.029294	C.017052
0.2	C.307701	C.249691	C.198415	C.154323	C.117434
0.3	C.459203	C.401947	C.347201	C.295849	C.248590
0.4	C.575098	C.521932	C.470925	C.420832	C.372366
0.5	C.659421	C.615327	C.570215	C.524640	C.479177
0.6	C.725783	C.688392	C.649466	C.609593	C.568609
0.7	C.777502	C.746054	C.712913	C.678350	C.642689
0.8	C.818291	C.791960	C.763970	C.734512	C.703826
0.9	C.850779	C.826789	C.805270	C.780355	C.754228
1.0	C.876865	C.858526	C.833827	C.811766	C.795775

TIME	CONCENTRATIONS AT GRID POINTS				
	11	12	13	14	15
0.1	0.005516	0.005093	0.002616	0.001290	0.000611
0.2	0.007402	0.006605	0.0045252	0.0031471	0.0021398
0.3	0.0205916	0.0168109	0.0135250	0.0107246	0.0083869
0.4	0.0326173	0.0282813	0.0242753	0.0206364	0.0173942
0.5	0.0434410	0.0390921	0.0349284	0.0310064	0.0273836
0.6	0.0527594	0.0486869	0.0447002	0.0408608	0.0372374
0.7	0.0606314	0.0569671	0.0533276	0.0497728	0.0463724
0.8	0.0672219	0.0640065	0.0607818	0.0576026	0.0545346
0.9	0.0727133	0.0699380	0.0671362	0.0643564	0.0616580
1.0	0.0772758	0.0749071	0.0725047	0.0701137	0.0677775

TIME	CONCENTRATIONS AT GRID POINTS				
	16	17	18	19	20
0.1	0.000279	0.000122	0.000052	0.000022	0.000010
0.2	0.0014255	0.0009292	0.0006013	0.0003991	0.0002991
0.3	0.0064807	0.0049727	0.0036341	0.0030504	0.0026323
0.4	0.0145736	0.0121999	0.0103064	0.0089441	0.0081936
0.5	0.0241207	0.0212859	0.0189617	0.0172540	0.0163038
0.6	0.0339075	0.0309620	0.0285105	0.0266881	0.0256670
0.7	0.0432085	0.0403791	0.0380028	0.0362248	0.0352243
0.8	0.0516571	0.0490661	0.0468776	0.0452332	0.0443055
0.9	0.0591137	0.0568122	0.0548611	0.0533911	0.0525604
1.0	0.0655696	0.0635662	0.0618637	0.0605785	0.0598515

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS TEN POINT GRID

TIME	1	2	3	4	5
0.1	0.422828	0.258009	0.137772	0.064546	0.026697
0.2	0.593431	0.456549	0.328045	0.219383	0.136324
0.3	0.696057	0.587523	0.474474	0.365750	0.268462
0.4	0.766702	0.679659	0.584407	0.486163	0.390461
0.5	0.817198	0.747259	0.668057	0.582660	0.494942
0.6	0.854755	0.798296	0.732727	0.659850	0.582250
0.7	0.883510	0.837042	0.783435	0.721053	0.654610
0.8	0.905861	0.868465	0.823660	0.771940	0.714439
0.9	0.923492	0.892915	0.855901	0.812644	0.763899
1.0	0.937559	0.912506	0.881928	0.845850	0.804800

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	0.009825	0.003244	0.000968	0.000264	0.000074
0.2	0.078694	0.042244	0.021155	0.010055	0.005171
0.3	0.167402	0.124369	0.078790	0.048767	0.032864
0.4	0.302365	0.225848	0.163647	0.117839	0.091427
0.5	0.409111	0.329435	0.260139	0.205897	0.173220
0.6	0.503219	0.426677	0.357289	0.300992	0.266229
0.7	0.584220	0.514100	0.448810	0.394660	0.360715
0.8	0.653067	0.590740	0.531674	0.481959	0.450500
0.9	0.711154	0.656859	0.604776	0.560508	0.532317
1.0	0.759934	0.713293	0.660166	0.629550	0.604852

INTERPOLATED VALUES

TIME	1	2	3	4	5
0.1	0.404616	0.239432	0.121722	0.052782	0.019469
0.2	0.586309	0.446525	0.316479	0.207624	0.125567
0.3	0.694309	0.582638	0.467518	0.357379	0.259427
0.4	0.766562	0.677447	0.580366	0.480581	0.383708
0.5	0.817756	0.746279	0.665597	0.578850	0.469947
0.6	0.855432	0.797724	0.730971	0.656971	0.578347
0.7	0.885891	0.837016	0.781837	0.719355	0.651248
0.8	0.906808	0.867533	0.821903	0.769413	0.711219
0.9	0.922944	0.891551	0.853785	0.809855	0.760537
1.0	0.936566	0.910657	0.879363	0.842674	0.801118

TIME	6	7	8	9	10
0.1	0.006113	0.001639	0.000375	0.000077	0.000013
0.2	0.069804	0.035606	0.016664	0.007243	0.003347
0.3	0.178397	0.116042	0.071573	0.042772	0.027849
0.4	0.294868	0.218052	0.155956	0.110555	0.084676
0.5	0.403167	0.322818	0.253157	0.198680	0.166506
0.6	0.498428	0.421186	0.351345	0.294914	0.260401
0.7	0.580125	0.509428	0.443786	0.389559	0.355903
0.8	0.649250	0.586521	0.527238	0.477567	0.446451
0.9	0.707345	0.652759	0.600563	0.556455	0.528648
1.0	0.755879	0.709037	0.663901	0.625486	0.601178

ASSOCIATED ERRORS

TIME	1	2	3	4	5
0.1	-0.018212	-0.018577	-0.016050	-0.011764	-0.007228
0.2	-0.007122	-0.010024	-0.011556	-0.011759	-0.010757
0.3	-0.002288	-0.004885	-0.006956	-0.008371	-0.009055
0.4	-0.000200	-0.002212	-0.004041	-0.005582	-0.006753
0.5	0.000556	-0.000980	-0.002460	-0.003816	-0.004995
0.6	0.000637	-0.000572	-0.001756	-0.002879	-0.003903
0.7	0.000375	-0.000626	-0.001598	-0.002516	-0.003362
0.8	-0.000053	-0.000932	-0.001765	-0.002535	-0.003220
0.9	-0.000548	-0.001364	-0.002116	-0.002789	-0.003362
1.0	-0.001053	-0.001849	-0.002564	-0.003184	-0.003688

ASSOCIATED ERRORS

TIME	6	7	8	9	10
0.1	-0.003712	-0.001605	-0.000593	-0.000187	-0.000061
0.2	-0.008890	-0.006638	-0.004491	-0.002812	-0.001824
0.3	-0.009005	-0.008327	-0.007217	-0.005995	-0.005015
0.4	-0.007497	-0.007796	-0.007691	-0.007284	-0.006751
0.5	-0.005944	-0.006617	-0.006982	-0.007017	-0.006714
0.6	-0.004791	-0.005491	-0.005944	-0.006078	-0.005828
0.7	-0.004095	-0.004672	-0.005032	-0.005101	-0.004812
0.8	-0.003817	-0.004219	-0.004436	-0.004392	-0.004049
0.9	-0.003509	-0.004099	-0.004193	-0.004053	-0.003669
1.0	-0.004055	-0.004255	-0.004265	-0.004064	-0.003674

APPENDIX C

TWO DIMENSIONAL HOMOGENEOUS CASE

The partial differential equation describing the problem is

$$\frac{\partial c}{\partial \theta} = \alpha \left[\frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} + \frac{\gamma \beta}{R} \frac{\partial}{\partial R} \left(R \frac{\partial c}{\partial R} \right) \right] .$$

$$0 < z < 1$$

$$0 \leq z \leq 1$$

The boundary conditions are:

$$(a) \quad \text{at } z = 0, \quad c = 1$$

$$\text{at } z = 1, \quad \frac{\partial c}{\partial z} = 0$$

$$\text{at } R = 0, \quad \frac{\partial c}{\partial R} = 0 \quad (\text{Radial Symmetry})$$

$$\text{at } R = 1, \quad \frac{\partial c}{\partial R} = 0 \quad (\text{No flow across the wall})$$

$$(b) \quad \text{at } z = 0, \quad c_{in}(\theta) = c_{z \rightarrow 0^+} - \alpha \left(\frac{\partial c}{\partial z} \right)_{z \rightarrow 0^+}$$

$$\text{at } z = 1, \quad \frac{\partial c}{\partial z} = 0$$

$$\text{at } R = 0, \quad \frac{\partial c}{\partial R} = 0$$

$$\text{at } R = 1, \quad \frac{\partial c}{\partial R} = 0.$$

Semi Analytical Solution A thirty point grid has been used for this problem. Because of the radial symmetry only the upper half of the reactor has been used for discretisation. The grid spacing is shown in Figure III-d.

No analytical solution is available for this type of problem.


```

C      SOLUTION OF THE DISPERSION MODEL EQUATION-TWO
C      DIMENSIONAL HOMOGENEOUS CASE
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
      REAL*8 DX,A
      DOUBLE PRECISION MATRIX(60,60),VECTOR(60,60),
1TOLERC,W(60,60),CEVR(60,60),TIME(60),CONC(15,10)
      DOUBLE PRECISION X(60),VAR(60),CI(60),C1(60)
      DOUBLE PRECISION D(60,60),VICTOR(60,60),R(15),
1SUM(15,10),CEVR1(15,10),DEV(15,10),DEVP(15,10)
C      READ THE DATA
      READ( 5,1) N,NT
      READ(5,5) ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 ) (CI(J),J=1,N)
      READ( 5,2 ) (C1(J),J=1,N)
      READ(5,3) (TIME(J), J=1,NT)
      READ(5,4) DX
      DO 99 J=1,NT
      READ(5,12) (CONC(J,K),K=1,5)
99  CONTINUE
      R(1)=0.0
      READ(5,6) (R(I),I=2,6)
      NORM=2
      TOLERC=0.000
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,220)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,223)
      WRITE(6,233)
      CALL LINECT(LINES,2,2)
      WRITE(6,234) (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,2,2)
      DO 30 J=1,N
30  C1(J)=C1(J)/(DX**2)
      WRITE(6,234) (C1(J),J=1,N)
      DO 36 J=1,N

```



```

DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(DX**2)
36 CONTINUE
WRITE(6,220)
WRITE(6,240)
CALL LINECT(LINES,4,2)
DO 31 J=1,15
WRITE(6,241)(MATRIX(J,K),K=1,N)
31 CONTINUE
WRITE(6,220)
DO 62 J=16,30
WRITE(6,241)(MATRIX(J,K),K=1,N)
62 CONTINUE
CALL TRANS(N,DX,D,MATRIX)
WRITE(6,255)
CALL LINECT(LINES,1,2)
WRITE(6,241)(D(J,J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,220)
WRITE(6,261)
DO 50 J=1,15
WRITE(6,241)(MATRIX(J,K),K=1,N)
50 CONTINUE
WRITE(6,220)
DO 63 J=16,30
WRITE(6,241)(MATRIX(J,K),K=1,N)
63 CONTINUE
CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NORM)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,6,2)
WRITE(6,242)
WRITE(6,232)(MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,243)
DO 32 K=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232)(VECTOR(K,J),J=1,N)
32 WRITE(6,223)
CALL CHECK(VECTOR,MATRIX,N,W)
CALL LINECT(LINES,1,2)
WRITE(6,223)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232)(W(J,K),K=1,N)
33 WRITE(6,223)
C CALCULATE THE TRANSPOSE OF THE MATRIX OF
C THE EIGENVECTORS

```



```

DO 40 I=1,N
DO 40 J=1,N
VICTOR(I,J)=VECTOR(J,I)
40 CONTINUE
C   A=(D(-1)*A(*)*D)
C   A(*)=THE ORIGINAL COEFFICIENT MATRIX
C   D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C   OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C   A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C   COEFFICIENT MATRIX A(*)
C   Q=THE MATRIX OF EIGENVECTORS OF A
C   CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C   COEFFICIENT MATRIX
DO 38 I=1,N
DO 38 J=1,N
VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
WRITE(6,220)
LINES=9
CALL LINECT(LINES,6,2)
WRITE(6,256)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,257)
DO 39 K=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
C   (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
C   QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
C   D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
C   CALCULATE THE PRODUCT (QT*D(-1))
DO 41 I=1,N
DO 41 J=1,N
VICTOR(I,J)=VICTOR(I,J)/D(J,J)
41 CONTINUE
CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
1CEVR,VICTOR)
WRITE(6,220)
WRITE(6,225)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,248)
DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)
WRITE(6,249)

```



```

      DO 35 J=1,NT
35  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=6,10 )
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,259)
      DO 45 J=1,NT
45  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=11,15)
      WRITE(6,220)
      WRITE(6,246)
      WRITE(6,260)
      DO 46 J=1,NT
46  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=16,20)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,265)
      DO 60 J=1,NT
60  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=21,25)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,266)
      DO 61 J=1,NT
61  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=26,30)
      SUM1=0.0
      DO 9 I=1,6
      SUM1=SUM1+R(I)
9  CONTINUE
      DO 8 J=1,NT
      DO 8 K=1,5
      SUM(J,K)=R(1)*CEVR(J,K)+R(2)*CEVR(J,K+5)
      1+R(3)*CEVR(J,K+10)+R(4)*CEVR(J,K+15)
      2+R(5)*CEVR(J,K+20)+R(6)*CEVR(J,K+25)
      CEVR1(J,K)=SUM(J,K)/SUM1
8  CONTINUE
      DO 10 J=1,NT
      DO 10 K=1,5
      DEV(J,K)=CEVR1(J,K)-CONC(J,K)
10 CONTINUE
      A=100.0
      DO 16 K=1,5
      DEVP(1,K)=0.0
16 CONTINUE
      DO 11 J=2,NT
      DO 11 K=1,5
      DEVP(J,K)=(DEV(J,K)/CEVR1(J,K))*A
11 CONTINUE
      WRITE(6,220)
      WRITE(6,270)
      WRITE(6,223)
      WRITE(6,248)
      DO 7 J=1,NT

```



```

      WRITE(6,251)    TIME(J), (CONC(J,K),K=1,5)
7  CONTINUE
      WRITE(6,223)
      WRITE(6,271)
      WRITE(6,248)
      DO 15 J=1,NT
      WRITE(6,251)    TIME(J), (CEVR1(J,K),K=1,5)
15 CONTINUE
      WRITE(6,220)
      WRITE(6,272)
      WRITE(6,223)
      WRITE(6,248)
      DO 13 J=1,NT
      WRITE(6,251)    TIME(J), (DEV(J,K),K=1,5)
13 CONTINUE
      WRITE(6,273)
      WRITE(6,223)
      WRITE(6,248)
      DO 14 J=1,NT
      WRITE(6,251)    TIME(J), (DEVP(J,K),K=1,5)
14 CONTINUE

```

C

FORMAT STATEMENTS

```

1  FORMAT(1X,2I4)
2  FORMAT(10F8.5)
3  FORMAT(11F7.3)
4  FORMAT(1X,F16.8)
5  FORMAT(10F8.5)
6  FORMAT(1X,F13.8,4F14.8)
12 FORMAT(5F16.6)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-TWO-,
      111HDIMENSIONAL/25X,22HNON HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,19HUSING ORDINARY B.C.)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,19H COEFFICIENT MATRIX)
241 FORMAT(1H,5X,10F6.2)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
      12H 3, 8X, 2H 4, 8X, 2H 5)

```



```
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,  
18X,2H 9, 8X, 2H10)  
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)  
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)  
255 FORMAT(1H,10X,9HMATRIX(D)/10X,  
119H(DIAGONAL ELEMENTS))  
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,  
127HORIGINAL COEFFICIENT MATRIX)  
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,  
127HORIGINAL COEFFICIENT MATRIX)  
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,  
18X,2H14,8X,2H15)  
260 FORMAT(1H,15X,5H TIME,9X,2H16,8X,2H17,8X,2H18,  
18X,2H19,8X,2H20)  
261 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX/  
120X,26H(CONVERTED INTO SYMMETRIC))  
265 FORMAT(1H,15X,5H TIME,9X,2H21,8X,2H22,8X,2H23,  
18X,2H24,8X,2H25)  
266 FORMAT(1H,15X,5H TIME,9X,2H26,8X,2H27,8X,2H28,  
18X,2H29,8X,2H30)  
270 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,  
111HDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)  
271 FORMAT(1H,10X,16HWEIGHTED AVERAGE/  
110X,32HTWO DIMENSIONAL HOMOGENEOUS CASE)  
272 FORMAT(1H,20X,18HABSOLUTE DEVIATION)  
273 FORMAT(1H,20X,17HPERCENT DEVIATION)  
STOP  
END
```


SUBROUTINE TRANS(N,DX,D,MATRIX)

THIS SUBROUTINE CONVERTS THE ORIGINAL COEFFICIENT
MATRIX TO THE REAL SYMMETRIC FORM USING
SIMILARITY TRANSFORMATION

INPUT DATA

DX= THE GRID SPACING

N= THE NUMBER OF GRID POINTS

D=THE DIAGONAL MATRIX ,WITH DIAGONAL ENTERIES

HAVING ALTERNATE SIGNS I.E. $D(I,I)=(-1)**(I)(D(I,I))$

USED FOR SIMILARITY TRANSFORMATION

MATRIX= THE ORIGINAL COEFFICIENT MATRIX (DIAGONALLY
DOMINANT & UNSYMMETRIC), DESTROYED DURING
COMPUTATION AND THE RESULTANT MATRIX IS SYMMETRIC
AND DIAGONALLY DOMANANT.

REAL*8 DX,ALPHA,BETA

DOUBLE PRECISION D(60,60),MATRIX(60,60)

ALPHA=0.2

BETA=DX/2.0

D(1,1)=1.0

CALCULATE THE DIAGONAL ELEMENTS OF MATRIX D.

DO 100 I=1,4

II=I+1

D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))

100 CONTINUE

D(6,6)=0.3535

DO 101 I=6,9

II=I+1

D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))

101 CONTINUE

D(11,11)=0.24995

DO 102 I=11,14

II=I+1

D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))

102 CONTINUE

D(16,16)=0.20408

DO 103 I=16,19

II=I+1

D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))

103 CONTINUE

D(21,21)=0.17673

DO 104 I=21,24

II=I+1

D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))

104 CONTINUE

D(26,26)=0.15807

DO 105 I=26,29

II=I+1

D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))

105 CONTINUE

DO 106 I=1,30,2

D(I,I)=-D(I,I)

106 CONTINUE

C
C CALCULATE THE COEFFICIENT MATRIX CONVERTED INTO
C THE SYMMETRIC ONE
C

DO 107 I=1,N

DO 107 J=1,N

MATRIX(I,J)=(MATRIX(I,J)*D(J,J))/(D(I,I))

107 CONTINUE

RETURN

END

CONCENTRATION PROFILES-TWO-DIMENSIONAL HOMOGENEOUS MEDIUM

INITIAL CONDITION VECTOR

[illegible]

BOUNDARY CONDITION VECTOR

[illegible]

COEFFICIENT MATRIX

[illegible]

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-1.20	0.0	0.0	0.0	0.0	14.98	-3.30	0.0	0.0	0.0
-1.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	-1.20	0.0	0.0	0.0	-8.80	14.98	-3.30	0.0	0.0
0.0	-1.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	-1.20	0.0	0.0	0.0	-8.80	14.98	-3.30	0.0
0.0	0.0	-1.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	-1.20	0.0	0.0	0.0	-8.80	14.98	-3.30
0.0	0.0	0.0	-1.68	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	-1.20	0.0	0.0	0.0	-8.80	11.68
0.0	0.0	0.0	0.0	-1.68	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	-1.26	0.0	0.0	0.0	0.0
14.98	-3.30	0.0	0.0	0.0	-1.62	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	-1.26	0.0	0.0	0.0
-8.80	14.98	-3.30	0.0	0.0	0.0	-1.62	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.26	0.0	0.0
0.0	-8.80	14.98	-3.30	0.0	0.0	0.0	-1.62	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.26	0.0
0.0	0.0	-8.80	14.98	-3.30	0.0	0.0	0.0	-1.62	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.26
0.0	0.0	0.0	-8.80	11.68	0.0	0.0	0.0	0.0	-1.62
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.29	0.0	0.0	0.0	0.0	13.40	-3.30	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	-1.29	0.0	0.0	0.0	-8.80	13.40	-3.30	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	-1.29	0.0	0.0	0.0	-8.80	13.40	-3.30	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	-1.29	0.0	0.0	0.0	-8.80	13.40	-3.30
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	-1.29	0.0	0.0	0.0	-8.80	10.10

MATRIX(D)

(DIAGONAL ELEMENTS)

1.00	1.63	-2.67	4.35	-7.11	0.35	-0.58	0.94	-1.54	2.51
0.25	0.41	-0.67	1.09	-1.78	0.20	-0.33	0.54	-0.89	1.45
0.18	0.29	-0.47	0.77	-1.26	0.16	-0.26	0.42	-0.69	1.12

ORIGINAL COEFFICIENT MATRIX
(CONVERTED INTO SYMMETRIC)

[illegible]

[illegible]

EIGENVALUES

28.210664	2.330177	3.001133	23.811465	26.401685
13.121033	18.038691	17.515409	4.379530	11.071680
12.688814	24.960273	23.293006	10.879835	5.721803
9.297188	18.893807	21.914608	6.045797	22.002486
16.229712	6.392759	20.561074	21.243653	7.488209
14.788300	7.771156	9.438423	16.844454	11.742635

EIGENVECTORS

0.263625	-0.021003	0.051527	-0.445306	-0.081612
-0.168749	-0.489913	0.119044	-0.066391	0.053385
-0.388916	0.098114	0.090805	-0.120399	-0.042379
0.192747	0.153384	-0.070475	0.071735	0.137857
0.151666	0.103969	-0.165731	-0.028727	-0.059670
-0.182333	0.133961	-0.144744	0.048524	0.130969

0.447083	0.038079	-0.093420	-0.391756	-0.138407
0.032273	0.093696	0.104728	0.120368	-0.010210
0.460394	0.166393	0.153996	0.142528	0.050168
-0.349454	0.134939	-0.119519	-0.130058	0.121279
-0.029006	-0.123078	-0.145801	-0.048718	0.108183
0.034871	-0.158581	0.171347	0.042689	-0.025048

0.494588	-0.048035	0.117845	0.100660	-0.153113
0.162576	0.471993	-0.026910	-0.151839	-0.051432
-0.156094	0.184073	0.170359	-0.048323	-0.017009
0.440822	-0.034672	-0.132219	0.164062	-0.031162
-0.146118	0.041729	0.037463	-0.053894	-0.136468
0.175663	0.053766	-0.058094	-0.010969	-0.126178

0.391693	0.049010	-0.120236	0.480312	-0.121259
-0.063366	-0.183965	-0.128402	0.154920	0.020046
-0.275612	0.145778	0.134917	-0.085323	-0.030033
-0.449765	-0.165442	-0.104712	-0.167391	-0.148694
0.056951	0.073680	0.178759	-0.042682	0.139237
-0.068467	0.094933	-0.102575	-0.052339	0.049180

0.169688	-0.040821	0.100145	0.321892	-0.052532
-0.150457	-0.436810	-0.086052	-0.129034	0.047598
0.482360	0.063153	0.058448	0.149328	0.052562
0.374612	-0.110874	-0.045363	0.139421	-0.099650
0.135226	-0.128950	0.119800	-0.018491	-0.115972
-0.162569	-0.166147	0.179522	-0.035076	0.116773

0.156906	0.059405	-0.128749	-0.265041	0.023972
0.307346	-0.291590	-0.297451	0.120920	-0.150992
-0.231478	-0.098314	-0.165385	0.035366	0.119864
0.114721	-0.279362	0.176093	-0.071882	-0.040493
-0.044550	-0.259784	0.166069	0.081249	0.017527
0.182704	-0.243986	0.145039	-0.137244	-0.327247

..CONTD

0.266099	-0.107702	0.233425	-0.233168	0.040655
-0.058780	0.055767	-0.261681	-0.219230	0.028877
0.274021	-0.166732	-0.280477	-0.041865	-0.141894
-0.207991	-0.245768	0.298638	0.130323	-0.035624
0.008520	0.307529	0.145099	0.137792	-0.031777
-0.034942	0.238828	-0.171696	-0.120740	0.062586

0.294373	0.135862	-0.294456	0.059912	0.044975
-0.296104	0.230925	0.067238	0.276549	0.145469
-0.092905	-0.184448	-0.310279	0.014194	0.048108
0.262372	0.063149	0.332370	-0.164397	0.009153
0.042920	-0.104266	-0.037540	0.152433	0.040086
-0.176022	-0.097925	0.058213	0.031024	0.315277

0.233131	-0.138618	0.300429	0.285876	0.035618
0.115410	-0.109494	0.320834	-0.282160	-0.056698
-0.164041	-0.146075	-0.245728	0.025062	0.084944
-0.267695	0.301323	0.261639	0.167732	0.043677
-0.016729	-0.184100	-0.179124	0.120720	-0.040899
0.068607	-0.172905	0.102785	0.148033	-0.122883

0.100996	0.115456	-0.250230	0.191586	0.015430
0.274032	-0.259984	0.215014	0.235013	-0.134625
0.287095	-0.063282	-0.106453	-0.043863	-0.148664
0.222965	0.201938	0.113346	-0.139705	0.029271
-0.039721	0.322202	-0.120044	0.052298	0.034065
0.162901	0.302608	-0.179888	0.099207	-0.291776

0.068884	-0.084006	0.117460	-0.116356	0.144630
0.058166	-0.128012	0.271369	0.022884	0.213521
-0.101622	-0.184849	-0.031299	0.213368	-0.169503
0.050364	-0.052870	-0.160653	-0.135151	-0.244305
-0.268777	0.237005	0.312241	-0.114897	0.105745
0.343518	-0.046175	0.272701	0.194080	0.298552

0.116821	0.152305	-0.212957	-0.102364	0.245280
-0.011124	0.024482	0.238736	-0.041490	-0.040836
0.120299	-0.313487	-0.053081	-0.252583	0.200656
-0.091311	-0.046512	-0.272452	0.245031	-0.214926
0.051404	-0.280564	0.274693	-0.194855	-0.191719
-0.065698	0.054661	-0.322820	0.170741	-0.057098

0.129233	-0.192126	0.268636	0.026302	0.271342
-0.056038	0.123329	-0.061342	0.052337	-0.205711
-0.040787	-0.346797	-0.058721	0.085637	-0.068031
0.115184	0.011951	-0.301402	-0.309097	0.055225
0.258946	0.095123	-0.070581	-0.215559	0.241845
-0.330953	-0.018532	0.109450	-0.043871	-0.287632

0.102347	0.106023	-0.274086	0.125503	0.214892
0.021842	-0.048069	-0.292701	-0.053399	0.080179

-0.072016	-0.24649	-0.045504	0.151207	-0.120121
-0.117521	0.057026	-0.238697	0.315368	0.263510
-0.100928	0.167958	-0.336786	-0.170714	-0.246751
0.128993	-0.032722	0.193254	-0.209337	0.112108

..CONTD

0.044339	-0.163269	0.228288	0.084109	0.093095
0.051861	-0.114136	-0.196160	0.044476	0.190377
0.126038	-0.118982	-0.020146	-0.264634	0.210230
0.097884	0.038217	-0.103408	-0.262672	0.176597
-0.239644	-0.293950	-0.225705	-0.073956	0.205521
0.306283	0.057269	-0.338223	-0.140292	0.266191

0.028732	0.102875	-0.042702	-0.048533	0.199637
-0.352215	-0.053395	-0.098655	-0.138573	-0.261482
-0.042387	-0.003401	0.189529	0.294518	0.207576
0.021007	0.320146	0.058404	-0.002487	-0.337221
-0.371000	-0.086162	0.005745	0.140705	0.145963
0.006320	0.279605	0.005017	-0.237674	-0.108537

0.048727	-0.186515	0.077419	-0.042697	0.338567
0.067361	0.010212	-0.086791	0.251235	0.050009
0.050178	-0.005768	0.321424	-0.348647	-0.245727
-0.038086	0.281647	0.099049	0.004508	-0.296669
0.070954	0.101997	0.005054	0.238622	-0.264634
-0.001209	-0.330994	-0.005939	-0.209093	0.020758

0.053904	0.235280	-0.097661	0.010971	0.374541
0.339332	0.051442	0.022301	-0.316922	0.251917
-0.017012	-0.006381	0.355577	0.118207	0.083312
0.048044	-0.072368	0.109573	-0.005687	0.076228
0.357430	-0.034582	-0.001299	0.263977	0.333825
-0.006089	0.112221	0.002014	0.053726	0.104567

0.042690	-0.240054	0.099643	0.052348	0.296621
-0.132259	-0.020050	0.106410	0.323352	-0.098188
-0.030038	-0.005053	0.281602	0.208715	0.147103
-0.049019	-0.345313	0.086777	0.005802	0.363730
-0.139313	-0.061060	-0.006196	0.209059	-0.340598
0.002373	0.198147	0.003556	0.256357	-0.040756

0.018494	0.199942	-0.082993	0.035082	0.128501
-0.314038	-0.047607	0.071313	-0.269322	-0.233139
0.052572	-0.002189	0.121995	-0.365281	-0.257451
0.040828	-0.231419	0.037593	-0.004833	0.243762
-0.330787	0.106864	-0.004153	0.090568	0.283686
0.005635	-0.346786	-0.006223	0.171804	-0.096772

0.011229	-0.118787	-0.053841	-0.018968	0.167021
0.141967	-0.020868	-0.124390	0.055854	0.301925
-0.018566	0.184786	-0.076393	0.246400	-0.239682
0.008210	-0.129041	0.073640	0.135105	-0.282126
-0.310387	-0.108638	-0.312134	-0.162468	0.122116
-0.343401	-0.112700	-0.272608	0.274435	-0.136850

0.019044	0.215363	0.097615	-0.016687	0.283252
-0.027151	0.003921	-0.102431	-0.101265	-0.057743

0.019611	0.313380	-0.129556	-0.291685	0.283733
-0.014885	-0.113523	0.124886	-0.244948	-0.248199
0.059362	0.128604	-0.274599	-0.275530	-0.221399
0.065676	0.133413	0.322710	0.241433	0.026173

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0.021067	-0.271671	-0.123137	0.004288	0.313349
-0.136774	0.020105	0.028118	0.127741	-0.290882
-0.006649	0.346678	-0.143322	0.098894	-0.096198
0.018777	0.029169	0.138156	0.308991	0.063774
0.299034	-0.043602	0.070557	-0.304807	0.279285
0.330840	-0.045233	-0.109413	-0.062035	0.131844

0.016684	0.277183	0.125635	0.020459	0.248159
0.053309	-0.007836	0.134168	-0.130333	0.113375
-0.011740	0.274555	-0.113505	0.174615	-0.169855
-0.019158	0.139185	0.109414	-0.315260	0.304304
-0.116552	-0.076988	0.336671	-0.241394	-0.284951
-0.128949	-0.079867	-0.193188	-0.296008	-0.051388

0.007228	-0.230868	-0.104642	0.013711	0.107507
0.126579	-0.018606	0.089916	0.108555	0.269199
0.020546	0.118942	-0.049172	-0.305602	0.297271
0.015957	0.093278	0.047400	0.262582	0.203936
-0.276743	0.134740	0.225628	-0.104576	0.237338
-0.306179	0.139778	0.338107	-0.198377	-0.122016

0.002866	0.132820	0.124945	-0.004842	0.062594
0.272414	-0.005326	0.288663	0.107176	-0.337594
-0.004228	0.110470	-0.146588	0.092343	0.267998
0.002096	-0.247611	-0.170891	0.080769	-0.105732
-0.116324	0.252109	-0.186603	0.181661	0.045765
-0.205295	-0.216255	-0.162972	-0.306856	0.317579

0.004861	-0.240806	-0.226529	-0.004259	0.106154
-0.052099	0.001019	0.253950	-0.194313	0.064565
0.005006	0.187347	-0.248599	-0.109315	-0.317253
-0.003799	-0.217835	-0.289815	-0.146437	-0.093018
0.022247	-0.298444	-0.164163	0.308081	-0.082974
0.039263	0.256001	0.192925	-0.269955	-0.060737

0.005377	0.303766	0.285756	0.001094	0.117434
-0.262450	0.005132	-0.065252	0.245118	0.325246
-0.001697	0.207254	-0.275014	0.037063	0.107563
0.004793	0.055972	-0.320609	0.184723	0.023901
0.112069	0.101186	0.042181	0.340816	0.104668
0.197786	-0.086796	-0.065410	0.069364	-0.305962

0.004259	-0.309929	-0.291554	0.005222	0.093003
0.102293	-0.002000	-0.311355	-0.250091	-0.126769
-0.002997	0.164136	-0.217800	0.065441	0.189921
-0.004890	0.267076	-0.253909	-0.188471	0.114044
-0.043680	0.178661	0.201271	0.269912	-0.106791
-0.077089	-0.153253	-0.115493	0.330978	0.119253

0.001845	0.258142	0.242837	0.003500	0.040290
0.242887	-0.004749	-0.208662	0.208302	-0.301001

0.005244	0.071107	-0.094354	-0.114530	-0.332390
0.004073	0.178987	-0.109998	0.156979	0.076429
-0.103715	-0.312683	0.134887	0.116930	0.088947
-0.183042	0.268215	0.202130	0.221812	0.283155

CHECK OF SIMILARITY TRANSFORMATION

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17.858331	5.390096	0.000000	-0.000000	-0.000000
2.035022	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000

5.390096	17.858331	5.390096	0.000000	0.000000
0.000000	2.035022	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	0.000000	-0.000000	-0.000000

0.000000	5.390096	17.858331	5.390096	0.000000
0.000000	0.000000	2.035022	0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	-0.000000	0.000000	-0.000000	-0.000000

-0.000000	0.000000	5.390096	17.858331	5.390096
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0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

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0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000

2.035022	0.000000	0.000000	-0.000000	-0.000000
14.980376	5.390096	-0.000000	0.000000	0.000000
1.526266	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000

0.000000	2.035022	0.000000	0.000000	0.000000
5.390096	14.980376	5.390096	0.000000	0.000000
-0.000000	1.526266	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	-0.000000

0.000000	-0.000000	2.035022	0.000000	0.000000
-0.000000	5.390096	14.980376	5.390096	-0.000000

0.000000	-0.000000	1.526266	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000
..CUMTD				
-0.000000	0.000000	0.000000	2.035022	-0.000000
0.000000	0.000000	5.390096	14.980376	5.390096
-0.000000	-0.000000	0.000000	1.526266	-0.000000
0.000000	0.000000	0.000000	-0.000000	0.000000
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0.000000	-0.000000	-0.000000	0.000000	0.000000
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0.000000	0.000000	-0.000000	5.390096	11.679441
-0.000000	-0.000000	-0.000000	-0.000000	1.526266
0.000000	0.000000	0.000000	-0.000000	-0.000000
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0.000000	0.000000	0.000000	-0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
1.526266	-0.000000	0.000000	-0.000000	-0.000000
14.980376	5.390096	-0.000000	0.000000	0.000000
1.468651	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
0.000000	1.526266	-0.000000	-0.000000	-0.000000
5.390096	14.980376	5.390096	0.000000	0.000000
-0.000000	1.468651	-0.000000	0.000000	0.000000
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-0.000000	0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	1.526266	0.000000	-0.000000
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0.000000	-0.000000	1.468651	0.000000	0.000000
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0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	1.526266	-0.000000
0.000000	0.000000	5.390096	14.980376	5.390096
-0.000000	-0.000000	0.000000	1.468651	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	1.526266
0.000000	0.000000	-0.000000	5.390096	11.679441
-0.000000	0.000000	0.000000	-0.000000	1.468651
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	2.000000

1.468651	-0.000000	0.000000	-0.000000	-0.000000
14.980376	5.390096	-0.000000	0.000000	-0.000000
1.453715	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000

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0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	1.468651	-0.000000	-0.000000	0.000000
5.390096	14.980376	5.390096	0.000000	0.000000
0.000000	1.453715	0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	0.000000

-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	1.468651	0.000000	0.000000
-0.000000	5.390096	14.980376	5.390096	-0.000000
0.000000	-0.000000	1.453715	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	1.468651	-0.000000
0.000000	0.000000	5.390096	14.980376	5.390096
-0.000000	0.000000	-0.000000	1.453715	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	1.468651
-0.000000	0.000000	-0.000000	5.390096	11.679441
-0.000000	0.000000	0.000000	-0.000000	1.453715
-0.000000	-0.000000	0.000000	0.000000	-0.000000

0.000000	0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
1.453715	0.000000	0.000000	-0.000000	-0.000000
14.980376	5.390096	-0.000000	0.000000	0.000000
1.447808	-0.000000	-0.000000	-0.000000	-0.000000

0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	1.453715	-0.000000	0.000000	0.000000
5.390096	14.980376	5.390096	0.000000	0.000000
-0.000000	1.447808	-0.000000	-0.000000	0.000000

-0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	1.453715	-0.000000	0.000000
-0.000000	5.390096	14.980376	5.390096	-0.000000
0.000000	-0.000000	1.447808	-0.000000	0.000000

0.000000	-0.000000	0.000000	0.000000	-0.000000
0.000000	-0.000000	-0.000000	0.000000	-0.000000

-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	1.453715	-0.000000
0.000000	0.000000	5.390096	14.980376	5.390096
-0.000000	-0.000000	0.000000	1.447808	-0.000000

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0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	1.453715
0.000000	0.000000	-0.000000	5.390096	11.679441
-0.000000	-0.000000	0.000000	-0.000000	1.447808

0.000000	0.000000	0.000000	0.000000	-0.000000
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-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
1.447808	-0.000000	0.000000	-0.000000	-0.000000
13.397379	5.390096	-0.000000	0.000000	0.000000

-0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	0.000000
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-0.000000	0.000000	-0.000000	0.000000	-0.000000
-0.000000	1.447808	-0.000000	-0.000000	-0.000000
5.390096	13.397379	5.390096	-0.000000	0.000000

-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	1.447808	0.000000	0.000000
-0.000000	5.390096	13.397379	5.390096	-0.000000

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	0.000000	-0.000000
0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	1.447808	-0.000000
0.000000	-0.000000	5.390096	13.397379	5.390096

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	1.447808
0.000000	0.000000	-0.000000	5.390096	10.696444

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

28.210664	2.330177	3.001133	23.811465	26.401685
13.121033	18.038691	17.515409	4.379530	11.071680
12.688814	24.960273	23.293006	10.879835	5.721803
9.297188	18.893807	21.914608	6.046797	22.002486
16.229712	6.392759	20.561074	21.243653	7.488209
14.788300	7.771156	9.438423	16.844454	11.742635

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.263625	0.021003	-0.051527	0.445306	0.081612
0.163749	0.489913	-0.119044	0.066391	-0.053385
0.388916	-0.098114	-0.090805	0.120399	0.042379
-0.192747	-0.153384	0.070475	-0.071735	-0.137857
-0.151666	-0.103969	0.165731	0.028727	0.059670
0.182333	-0.133961	0.144744	-0.048524	-0.130969

0.730042	0.062180	-0.152545	-0.639699	-0.226005
0.052699	0.152996	0.171011	0.196549	-0.016672
0.751777	0.271703	0.251460	0.232733	0.081920
-0.570624	0.220342	-0.195163	-0.212371	0.198036
-0.047364	-0.200973	-0.238079	-0.079551	0.176652
0.056941	-0.258947	0.279792	0.069707	-0.040901

-1.318751	0.128080	-0.314218	-0.268397	0.408256
-0.433487	-1.258504	0.071751	0.404859	0.137137
0.416203	-0.490805	-0.454239	0.128847	0.045353
-1.175390	0.092448	0.352543	-0.437449	0.083090
0.389604	-0.111264	-0.099890	0.143702	0.363874
-0.468382	-0.143360	0.154900	0.029247	0.336437

1.705393	0.213384	-0.523496	2.091229	-0.527951
-0.275890	-0.800966	-0.559050	0.674506	0.087280
-1.199986	0.634703	0.587416	-0.371489	-0.130760
-1.958232	-0.720316	-0.455904	-0.728803	-0.647397
0.247961	0.320793	0.778301	-0.185833	0.606225
-0.298099	0.413331	-0.446603	-0.227877	0.214123

-1.206393	0.290214	-0.711982	-2.288484	0.373472
1.069675	3.105490	0.611782	0.917364	-0.338399
-3.429331	-0.448988	-0.415538	-1.061644	-0.373687
-2.663300	0.788250	0.322506	-0.991211	0.708463
-0.961390	0.916766	-0.851714	0.131458	0.824498
1.155782	1.181221	-1.276307	0.249371	-0.830193

0.055475	0.021003	-0.045520	-0.093706	0.008476
0.108663	-0.103093	-0.105165	0.042752	-0.053384
-0.081840	-0.034759	-0.053472	0.012504	0.042378
0.040560	-0.098770	0.062258	-0.025414	-0.014317
-0.015751	-0.091847	0.058714	0.028726	0.006197
0.064596	-0.086262	0.051279	-0.048523	-0.115699

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-0.153623	0.062178	-0.134760	0.134612	-0.023471
0.033935	-0.032195	0.151073	0.126565	-0.016671
-0.158197	0.096257	0.161924	0.024170	0.081918
0.120077	0.141886	-0.172409	-0.075238	0.020566
-0.004919	-0.177542	-0.084345	-0.079550	0.018346
0.020173	-0.166745	0.099123	0.069705	-0.036132

0.277506	0.128077	-0.277584	0.056479	0.042398
-0.279138	0.264828	0.063385	0.260703	0.137134
-0.087582	-0.173879	-0.292501	0.013381	0.045352
0.247338	0.059531	0.311440	-0.154977	0.008629
0.040461	-0.098292	-0.035389	0.143699	0.037789
-0.165936	-0.092314	0.054877	0.029246	0.297212

-0.358867	0.213380	-0.462462	-0.440059	-0.054828
-0.177655	0.168548	-0.493871	0.434339	0.087278
0.252514	0.224859	0.378259	-0.038580	-0.130757
0.412072	-0.463838	-0.402751	-0.258196	-0.067233
0.025751	0.283392	0.275732	-0.185829	0.062957
-0.105609	0.266159	-0.158220	-0.227872	0.189159

0.253862	0.290208	-0.628973	0.481567	0.038786
0.688802	-0.653490	0.540455	0.590724	-0.338392
0.721637	-0.159065	-0.267580	-0.110253	-0.373679
0.560440	0.507589	0.284905	-0.351160	0.073575
-0.099842	0.809881	-0.301740	0.131455	0.085625
0.409464	0.760630	-0.452163	0.249366	-0.733402

-0.017221	0.021001	-0.029365	0.029089	-0.036158
-0.014541	0.032003	-0.067842	-0.005721	-0.053380
0.025405	0.046212	0.007825	-0.053342	0.042376
-0.012591	0.013217	0.040163	0.033788	0.061076
0.067194	-0.059251	-0.078060	0.028724	-0.026436
-0.085880	0.011544	-0.068175	-0.048520	-0.074638

0.047689	0.062175	-0.086934	-0.041787	0.100129
-0.004541	0.009994	0.097458	-0.016937	-0.016670
0.049109	-0.127973	-0.021669	-0.103111	0.081913
-0.037275	-0.018987	-0.111222	0.100028	-0.087738
0.020984	-0.114533	0.112136	-0.079545	-0.073264
-0.026820	0.022314	-0.131783	0.069701	-0.023309

-0.086146	0.128069	-0.179070	-0.017533	-0.180874
0.037354	-0.082210	0.040890	-0.034887	0.137125
0.027188	0.231171	0.039143	-0.057085	0.045349
-0.076781	-0.007966	0.200911	0.200041	-0.036812
-0.172611	-0.063408	0.047049	0.143690	-0.161211
0.220610	0.012354	-0.072959	0.029244	0.191733

0.111403	0.213367	-0.298336	0.136607	0.233904
0.023774	-0.052322	-0.318598	-0.058124	0.087272

-0.078388	-0.293948	-0.050619	0.164585	-0.130740
-0.127919	0.062071	-0.259816	0.343270	0.286824
-0.109857	0.182818	-0.366584	-0.185818	-0.268583
0.140406	-0.035518	0.210352	-0.227858	0.122027

..CONTD

-0.078806	0.290190	-0.405753	-0.149492	-0.165464
-0.092176	0.202862	0.348650	-0.079051	-0.338370
-0.224017	0.211475	0.035808	0.470352	-0.373656
-0.173977	-0.067926	0.183794	0.466865	-0.313878
0.425936	0.522458	0.401161	0.131447	-0.365287
-0.544379	-0.101788	0.601147	0.249350	-0.473121

0.005865	0.020999	-0.008716	-0.009907	0.040751
-0.071896	-0.010899	-0.020138	-0.028286	-0.053375
-0.008652	-0.000694	0.038687	0.060118	0.042371
0.004288	0.065350	0.011922	-0.000508	-0.068835
-0.075730	-0.017588	0.001173	0.028721	0.029795
0.001290	0.057074	0.001024	-0.048515	-0.022155

-0.016241	0.062168	-0.025805	0.014231	-0.112849
-0.022453	-0.003404	0.028929	-0.083740	-0.016669
-0.016725	0.001922	-0.107135	0.116209	0.081904
0.012695	-0.093877	-0.033014	-0.001503	0.098884
-0.023650	-0.033997	-0.001685	-0.079536	0.088206
0.000403	0.110325	0.001980	0.069694	-0.006919

0.029338	0.128056	-0.053154	0.005971	0.203851
0.184688	0.027998	0.012138	-0.172491	0.137111
-0.009259	-0.003473	0.193529	0.064336	0.045344
0.026149	-0.039388	0.059637	-0.003095	0.041489
0.194538	-0.018822	-0.000707	0.143675	0.181690
-0.003314	0.061079	0.001096	0.029241	0.056913

-0.037940	0.213344	-0.088556	-0.046524	-0.263618
0.117543	0.017819	-0.094571	-0.287375	0.087263
0.026696	0.004491	-0.250270	-0.185493	-0.130735
0.043565	0.306892	-0.077122	-0.005157	-0.323260
0.123813	0.054266	0.005507	-0.185798	0.302701
-0.002109	-0.176100	-0.003160	-0.227834	0.036222

0.026839	0.290160	-0.120441	0.050912	0.186483
-0.455737	-0.069088	0.103491	-0.390845	-0.338335
0.076293	-0.003177	0.177041	-0.530102	-0.373617
0.059251	-0.335840	0.054556	-0.007013	0.353751
-0.480043	0.155083	-0.006026	0.131433	0.411690
0.008178	-0.503261	-0.009031	0.249324	-0.140438

-0.001985	0.020999	0.009518	0.003353	-0.029525
-0.025096	0.003689	0.021989	-0.009874	-0.053373
0.002928	-0.032666	0.013505	-0.043558	0.042370
-0.001451	0.022811	-0.013018	-0.023883	0.049873
0.054869	0.019205	0.055178	0.028720	-0.021587
0.060705	0.019023	0.043101	-0.048514	0.024192

0.005497	0.062168	0.028177	-0.004817	0.081763
-0.007837	0.001152	-0.031588	-0.029231	-0.016668

0.005861	0.007460	-0.037397	-0.084197	0.081902
-0.004297	-0.032789	0.036049	-0.070706	-0.071645
0.017135	0.057123	-0.079265	-0.079534	-0.063909
0.018958	0.038511	0.093153	0.069692	0.007555

..CONID

-0.009930	0.128052	0.058041	-0.002021	-0.147697
0.064469	-0.009476	-0.013253	-0.060211	0.137107
0.003134	-0.163407	0.067555	-0.046614	0.045343
-0.008850	-0.013749	-0.065120	-0.145643	-0.030060
-0.140950	0.020552	-0.033257	0.143671	-0.131641
-0.155942	0.021321	0.051572	0.029240	-0.062145

0.012841	0.213339	0.096697	0.015747	0.191000
0.041031	-0.006031	0.103265	-0.100313	0.087261
-0.009036	0.211316	-0.087361	0.134396	-0.130732
-0.014745	0.107126	0.084212	-0.242645	0.234213
-0.089707	-0.059255	0.259125	-0.185793	-0.219318
-0.099248	-0.061471	-0.148691	-0.227828	-0.039552

-0.009084	0.290152	0.131513	-0.017232	-0.135113
-0.159083	0.023384	-0.113005	-0.136431	-0.338326
-0.025822	-0.149485	0.061799	0.384078	-0.373607
-0.020054	-0.117231	-0.059572	-0.330011	-0.256305
0.347808	-0.160340	-0.283567	0.131430	-0.293284
0.384803	-0.175672	-0.424930	0.249318	0.153349

0.000453	0.021001	0.019756	-0.000766	0.009897
0.043073	-0.000842	0.045642	0.016946	-0.053378
-0.000669	0.017467	-0.023178	0.014601	0.042374
0.000331	-0.039151	-0.027020	0.012771	-0.016718
-0.018392	0.039862	-0.029504	0.028723	0.007236
-0.032460	-0.034193	-0.025768	-0.048518	0.050214

-0.001255	0.062172	0.058486	0.001100	-0.027407
0.013451	-0.000263	-0.065566	0.050169	-0.016670
-0.001292	-0.048370	0.064184	0.028223	0.081910
0.000981	0.056242	0.074826	0.037808	0.024016
-0.005744	0.077053	0.042384	-0.079542	0.021422
-0.010137	-0.066095	-0.049810	0.069698	0.015681

0.002267	0.128064	0.120472	0.000461	0.049509
-0.110646	0.002163	-0.027509	0.103339	0.137120
-0.000715	0.087376	-0.115943	0.015625	0.045347
0.002021	0.023597	-0.135165	0.077877	0.010076
0.047247	0.042659	0.017783	0.143684	0.044127
0.083384	-0.036592	-0.027576	0.029243	-0.128990

-0.002932	0.213359	0.200709	-0.003595	-0.064024
-0.070420	0.001377	0.214340	0.172165	0.087269
0.002063	-0.112993	0.143936	-0.045050	-0.130744
0.003366	-0.183858	0.174794	0.129746	-0.078509
0.030070	-0.122993	-0.133558	-0.185811	0.073516
0.053069	0.105501	0.079507	-0.227849	-0.082095

0.002074	0.200179	0.272975	0.003934	0.045291
0.273031	-0.005339	-0.234558	0.234154	-0.338358

0.005895	0.071931	-0.106065	-0.128745	-0.373642
0.004578	0.201201	-0.123649	0.175461	0.035915
-0.116587	-0.351489	0.151627	0.131442	0.099986
-0.205759	0.301503	0.227216	0.249341	0.318297

SOLUTION OF THE DISPERSION MODELEQUATION
 USING ORDINARY B.C.
 SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528611	0.187828	0.049082	0.010054	0.001767
0.2	0.731448	0.419487	0.191837	0.072031	0.024547
0.3	0.828839	0.585768	0.350377	0.179528	0.086935
0.4	0.883289	0.698782	0.488202	0.302780	0.182271
0.5	0.916891	0.776617	0.598929	0.421872	0.293197
0.6	0.939042	0.831595	0.685664	0.527865	0.404750
0.7	0.954339	0.871396	0.753204	0.618159	0.507819
0.8	0.965272	0.900824	0.805844	0.693157	0.598226
0.9	0.973291	0.922956	0.846990	0.754488	0.674943
1.0	0.979290	0.939825	0.879250	0.804143	0.738646

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528611	0.187828	0.049082	0.010054	0.001767
0.2	0.731448	0.419487	0.191837	0.072031	0.024547
0.3	0.828839	0.585768	0.350377	0.179528	0.086935
0.4	0.883289	0.698781	0.488201	0.302779	0.182270
0.5	0.916891	0.776616	0.598928	0.421871	0.293197
0.6	0.939041	0.831594	0.685663	0.527864	0.404749
0.7	0.954339	0.871395	0.753202	0.618157	0.507817
0.8	0.965271	0.900823	0.805842	0.693154	0.598223
0.9	0.973290	0.922954	0.846988	0.754485	0.674939
1.0	0.979289	0.939823	0.879247	0.804140	0.738642

CONCENTRATIONS AT GRID POINTS

TIME	11	12	13	14	15
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528611	0.187828	0.049082	0.010054	0.001767
0.2	0.731447	0.419486	0.191836	0.072031	0.024547
0.3	0.828838	0.585766	0.350375	0.179527	0.086934
0.4	0.883287	0.698778	0.488198	0.302777	0.182269
0.5	0.916888	0.776612	0.598922	0.421866	0.293193
0.6	0.939038	0.831588	0.685655	0.527857	0.404743
0.7	0.954335	0.871388	0.753193	0.618147	0.507808
0.8	0.965268	0.900815	0.805832	0.693142	0.598211
0.9	0.973286	0.922946	0.846976	0.754471	0.674925
1.0	0.979285	0.939814	0.879233	0.804124	0.738625

CONCENTRATIONS AT GRID POINTS					
TIME	16	17	18	19	20
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528607	0.187826	0.049081	0.010054	0.001767
0.2	0.731438	0.419478	0.191832	0.072029	0.024547
0.3	0.828825	0.585751	0.350365	0.179521	0.086931
0.4	0.883271	0.698758	0.488181	0.302765	0.182261
0.5	0.916871	0.776587	0.598899	0.421847	0.293179
0.6	0.939019	0.831560	0.685626	0.527831	0.404722
0.7	0.954315	0.871357	0.753159	0.618115	0.507780
0.8	0.965247	0.900782	0.805794	0.693105	0.598176
0.9	0.973265	0.922911	0.846935	0.754429	0.674884
1.0	0.979263	0.939778	0.879190	0.804078	0.738578

CONCENTRATIONS AT GRID POINTS					
TIME	21	22	23	24	25
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528605	0.187825	0.049081	0.010054	0.001767
0.2	0.731434	0.419475	0.191830	0.072028	0.024546
0.3	0.828820	0.585746	0.350361	0.179518	0.086930
0.4	0.883265	0.698751	0.488175	0.302761	0.182258
0.5	0.916864	0.776579	0.598891	0.421841	0.293174
0.6	0.939012	0.831551	0.685617	0.527823	0.404715
0.7	0.954308	0.871347	0.753149	0.618106	0.507772
0.8	0.965239	0.900771	0.805782	0.693094	0.598167
0.9	0.973257	0.922900	0.846923	0.754417	0.674873
1.0	0.979255	0.939766	0.879177	0.804065	0.738567

CONCENTRATIONS AT GRID POINTS					
TIME	26	27	28	29	30
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528611	0.187828	0.049082	0.010054	0.001767
0.2	0.731447	0.419486	0.191836	0.072031	0.024547
0.3	0.828837	0.585766	0.350375	0.179526	0.086934
0.4	0.883287	0.698778	0.488198	0.302776	0.182268
0.5	0.916888	0.776611	0.598922	0.421866	0.293193
0.6	0.939038	0.831587	0.685655	0.527856	0.404742
0.7	0.954334	0.871387	0.753192	0.618146	0.507807
0.8	0.965267	0.900814	0.805830	0.693141	0.598210
0.9	0.973286	0.922945	0.846974	0.754469	0.674923
1.0	0.979284	0.939812	0.879232	0.804122	0.738622

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.528611	0.187829	0.049082	0.010054	0.001767
0.2	0.731448	0.419487	0.191837	0.072031	0.024547
0.3	0.823839	0.585768	0.350377	0.179528	0.086935
0.4	0.883290	0.698782	0.488202	0.302780	0.182271
0.5	0.916891	0.776618	0.598929	0.421872	0.293198
0.6	0.939042	0.831595	0.685665	0.527866	0.404751
0.7	0.954340	0.871397	0.753205	0.618160	0.507821
0.8	0.965273	0.900825	0.805846	0.693159	0.598228
0.9	0.973292	0.922958	0.846993	0.754491	0.674946
1.0	0.979291	0.939827	0.879253	0.804148	0.738651

WEIGHTED AVERAGE TWO DIMENSIONAL HOMOGENEOUS CASE

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528609	0.187827	0.049082	0.010054	0.001767
0.2	0.731442	0.419482	0.191834	0.072030	0.024547
0.3	0.828831	0.585758	0.350370	0.179523	0.086933
0.4	0.883279	0.698767	0.488189	0.302770	0.182264
0.5	0.916879	0.776599	0.598910	0.421856	0.293185
0.6	0.939028	0.831573	0.685640	0.527843	0.404732
0.7	0.954324	0.871372	0.753175	0.618131	0.507793
0.8	0.965257	0.900797	0.805812	0.693123	0.598193
0.9	0.973275	0.922927	0.846954	0.754449	0.674904
1.0	0.979273	0.939795	0.879211	0.804100	0.738601

ABSOLUTE DEVIATION

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	-0.000002	-0.000002	-0.000000	-0.000000	0.000000
0.2	-0.000006	-0.000005	-0.000003	-0.000001	-0.000000
0.3	-0.000008	-0.000010	-0.000007	-0.000005	-0.000002
0.4	-0.000011	-0.000015	-0.000013	-0.000010	-0.000007
0.5	-0.000012	-0.000019	-0.000019	-0.000016	-0.000013
0.6	-0.000014	-0.000022	-0.000025	-0.000023	-0.000019
0.7	-0.000016	-0.000025	-0.000030	-0.000029	-0.000028
0.8	-0.000016	-0.000028	-0.000034	-0.000036	-0.000035
0.9	-0.000017	-0.000031	-0.000039	-0.000042	-0.000042
1.0	-0.000018	-0.000032	-0.000042	-0.000048	-0.000050

PERCENT DEVIATION

TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	-0.000448	-0.000935	-0.000424	-0.002246	0.004335
0.2	-0.000756	-0.001278	-0.001675	-0.001952	-0.000448
0.3	-0.000998	-0.001706	-0.002079	-0.002609	-0.002532
0.4	-0.001275	-0.002108	-0.002682	-0.003228	-0.003589
0.5	-0.001338	-0.002479	-0.003184	-0.003767	-0.004272
0.6	-0.001489	-0.002634	-0.003658	-0.004319	-0.004777
0.7	-0.001638	-0.002901	-0.003926	-0.004747	-0.005476
0.8	-0.001699	-0.003080	-0.004263	-0.005226	-0.005869
0.9	-0.001752	-0.003315	-0.004603	-0.005554	-0.006296
1.0	-0.001801	-0.003444	-0.004832	-0.006001	-0.006808

CONCENTRATION PROFILES-TWO-DIMENSIONAL HOMOGENEOUS MEDIUM

INITIAL CONDITION VECTOR

[illegible]

BOUNDARY CONDITION VECTOR

[illegible]

COEFFICIENT MATRIX

[illegible]

COEFFICIENT MATRIX

...CONTD

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-1.20	0.0	0.0	0.0	0.0	10.37	-3.30	0.0	0.0	0.0
-1.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	-1.20	0.0	0.0	0.0	-8.80	14.98	-3.30	0.0	0.0
0.0	-1.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	-1.20	0.0	0.0	0.0	-8.80	14.98	-3.30	0.0
0.0	0.0	-1.68	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	-1.20	0.0	0.0	0.0	-8.80	14.98	-3.30
0.0	0.0	0.0	-1.68	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	-1.20	0.0	0.0	0.0	-8.80	11.68
0.0	0.0	0.0	0.0	-1.68	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	-1.26	0.0	0.0	0.0	0.0
10.37	-3.30	0.0	0.0	0.0	-1.62	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	-1.26	0.0	0.0	0.0
-8.80	14.98	-3.30	0.0	0.0	0.0	-1.62	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.26	0.0	0.0
0.0	-8.80	14.98	-3.30	0.0	0.0	0.0	-1.62	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.26	0.0
0.0	0.0	-8.80	14.98	-3.30	0.0	0.0	0.0	-1.62	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.26
0.0	0.0	0.0	-8.80	11.68	0.0	0.0	0.0	0.0	-1.62
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-1.29	0.0	0.0	0.0	0.0	8.79	-3.30	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	-1.29	0.0	0.0	0.0	-8.80	13.40	-3.30	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	-1.29	0.0	0.0	0.0	-8.80	13.40	-3.30	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	-1.29	0.0	0.0	0.0	-8.80	13.40	-3.30
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	-1.29	0.0	0.0	0.0	-8.80	10.10

MATRIX(D)

(DIAGONAL ELEMENTS)

-1.00	1.63	-2.67	4.35	-7.11	0.50	-0.82	1.33	-2.18	3.55
-0.35	0.58	-0.94	1.54	-2.51	0.29	-0.47	0.77	-1.26	2.05
-0.25	0.41	-0.67	1.09	-1.78	0.22	-0.37	0.60	-0.97	1.50

(CONVERTED INTO SYMMETRIC)

[illegible]

ORIGINAL COEFFICIENT MATRIX
(CONVERTED INTO SYMMETRIC)

...CONTD

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.47	0.0	0.0	0.0	0.0	10.37	5.39	0.0	0.0	0.0
1.45	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.47	0.0	0.0	0.0	5.39	14.98	5.39	0.0	0.0
0.0	1.45	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.47	0.0	0.0	0.0	5.39	14.98	5.39	0.0
0.0	0.0	1.45	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.47	0.0	0.0	0.0	5.39	14.98	5.39
0.0	0.0	0.0	1.45	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.47	0.0	0.0	0.0	5.39	11.68
0.0	0.0	0.0	0.0	1.45	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	1.45	0.0	0.0	0.0	0.0
10.37	5.39	0.0	0.0	0.0	1.45	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	1.45	0.0	0.0	0.0
5.39	14.98	5.39	0.0	0.0	0.0	1.45	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.45	0.0	0.0
0.0	5.39	14.98	5.39	0.0	0.0	0.0	1.45	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.45	0.0
0.0	0.0	5.39	14.98	5.39	0.0	0.0	0.0	1.45	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.45
0.0	0.0	0.0	5.39	11.68	0.0	0.0	0.0	0.0	1.45
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1.45	0.0	0.0	0.0	0.0	8.79	5.39	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	1.45	0.0	0.0	0.0	5.39	13.40	5.39	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	1.45	0.0	0.0	0.0	5.39	13.40	5.39	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	1.45	0.0	0.0	0.0	5.39	13.40	5.39
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	1.45	0.0	0.0	0.0	5.39	10.10

EIGENVALUES

1.716131	28.641549	4.303104	24.536127	11.402647
3.611228	26.084036	23.572911	16.294853	15.798000
2.212976	17.282477	21.363514	13.177036	4.799939
9.520517	17.693099	5.385614	22.761753	6.933535
6.198199	21.015395	9.491052	19.467480	9.507551
7.972591	20.866651	12.073038	14.724958	10.004393

EIGENVECTORS

0.100960	0.162936	-0.121315	-0.055861	0.152813
-0.141561	-0.040817	0.307993	0.112596	-0.080555
0.141122	-0.416708	0.059566	-0.142865	0.169607
-0.116069	0.112946	-0.132332	0.059751	-0.096699
0.170125	0.077154	0.386019	-0.105593	-0.109143
0.159045	-0.042620	-0.463900	-0.104391	0.152345

-0.106653	0.406773	0.069926	-0.139459	0.059464
0.149543	-0.101901	0.479286	0.175216	-0.125356
-0.149079	-0.162151	0.148706	-0.055592	-0.097772
0.067048	0.175761	0.139800	0.149169	0.102153
-0.098068	0.120062	-0.407788	-0.164319	-0.042313
-0.091679	-0.106399	0.267406	-0.240621	0.059278

0.102931	0.504649	0.021201	-0.173015	-0.180537
-0.144323	-0.126420	0.027896	0.010198	-0.007297
0.143877	0.492307	0.184485	0.168784	-0.029613
0.020125	0.010230	-0.134931	0.185061	-0.093592
-0.029710	0.006982	0.393561	-0.009564	0.128775
-0.027781	-0.131996	0.081032	0.123329	-0.179980

-0.090124	0.421442	-0.100285	-0.144488	0.024707
0.126366	-0.105576	-0.450736	-0.168069	0.120244
-0.125976	-0.067375	0.154066	-0.023099	0.140165
-0.096028	-0.168592	0.118151	0.154548	0.086328
0.140604	-0.115175	-0.344592	0.157617	-0.017739
0.131455	-0.110228	-0.383427	-0.016878	0.024634

0.069362	0.187010	0.122389	-0.064115	0.169018
-0.097254	-0.046848	-0.350084	-0.127982	0.091565
0.096955	-0.460896	0.068365	-0.158015	-0.171069
0.117388	-0.128381	-0.090937	0.068579	-0.066442
-0.171601	-0.087703	0.265206	0.120024	-0.120393
-0.160434	-0.048911	0.467951	-0.115460	0.168492

-0.204793	0.109672	0.246089	0.042086	-0.209349
0.193935	0.008799	0.207309	-0.208954	0.163402
-0.261896	-0.280485	-0.110540	0.107637	-0.314749
0.024754	-0.154730	0.099689	-0.081856	0.020840
-0.233060	-0.016628	0.259835	0.079555	0.221097
-0.119827	0.006448	-0.312249	0.022503	-0.282717

..CONTD

0.216339	0.273798	-0.141849	0.105070	-0.081462
-0.204868	0.021966	0.322606	-0.325166	0.254279
0.276662	-0.109144	-0.275966	0.041884	0.181436
-0.014554	-0.240785	-0.105320	-0.204354	-0.022018
0.134345	-0.025871	-0.274479	0.123800	0.086009
0.069072	0.215818	0.179991	0.008757	-0.112012

-0.208791	0.339678	-0.042998	0.130351	0.247328
0.197717	0.027251	0.018777	-0.018926	0.014800
-0.267009	0.331371	-0.342367	-0.127165	0.054966
-0.004028	-0.014015	0.101661	-0.253524	0.021253
0.040707	-0.001494	0.264898	0.007205	-0.261186
0.020931	0.267745	0.054542	-0.026585	0.334007

0.182812	0.283672	0.203417	0.108858	-0.033848
-0.173115	0.022758	-0.309447	0.311903	-0.243907
0.233787	-0.045350	-0.285917	0.017403	-0.260130
0.020659	0.230963	-0.089026	-0.211723	-0.018612
-0.192627	0.024837	-0.231942	-0.118751	0.035775
-0.099041	0.223598	-0.258084	0.003638	-0.045711

-0.140698	0.125876	-0.248255	0.048305	-0.231547
0.133233	0.010099	-0.235641	0.237511	-0.185732
-0.179930	-0.310227	-0.126872	0.119051	0.317479
-0.025598	0.175876	0.063525	-0.093950	0.014327
0.235091	0.018909	0.178515	-0.090427	0.244474
0.120874	0.099219	0.314977	0.024888	-0.312696

0.206773	0.038760	-0.248495	0.124902	-0.142105
0.131637	0.089980	0.073267	0.124880	-0.164981
0.156525	-0.099129	0.066060	0.319437	0.183090
0.256482	-0.105033	0.295916	-0.055566	0.213171
-0.158211	-0.170091	0.091826	0.236099	-0.222875
-0.355615	-0.037275	-0.110354	0.230125	0.168964

-0.218431	0.096765	0.143247	0.311821	-0.055297
-0.139061	0.224638	0.114015	0.194335	-0.256736
-0.165351	-0.038573	0.164922	0.124301	-0.108410
-0.147559	-0.163449	-0.312600	-0.138722	-0.225194
0.091204	-0.264692	-0.097009	0.367408	-0.087046
0.204987	-0.217890	0.063612	0.089547	0.065755

0.210809	0.120048	0.043389	0.386849	0.167886
0.134212	0.278689	0.006636	0.011311	-0.014942
0.159581	0.117112	0.204608	-0.377389	-0.032882
-0.045099	-0.009513	0.301590	-0.172101	0.217342
0.027619	-0.015417	0.093626	0.021384	0.263641
0.062117	-0.270328	0.019276	-0.271875	-0.199625

-0.184580	0.100255	-0.205364	0.223065	-0.022976
-0.117517	0.232738	-0.109364	-0.186408	0.246263

-0.139726	-0.026027	0.170875	0.051648	0.155501
0.211795	0.156782	-0.264152	-0.143725	-0.190305
-0.130742	0.253877	-0.681972	-0.352421	-0.035811
-0.293924	-0.225766	-0.091211	0.037208	0.027314

..CONID

0.142058	0.044487	0.250641	0.143357	-0.157175
0.090446	0.103275	-0.083280	-0.141948	0.187526
0.107538	-0.109640	0.075825	0.353310	-0.189771
-0.258098	0.119388	0.203299	-0.063776	0.146467
0.159569	0.193328	0.063083	-0.268364	-0.247214
0.358717	-0.100184	0.111319	0.254528	0.186896

-0.203890	0.013104	0.245035	0.016618	0.320585
-0.296966	0.129173	0.024770	0.007722	0.162675
0.009674	-0.033513	0.004087	0.042494	0.011620
0.367486	0.236945	0.039385	0.125350	0.306039
0.356878	-0.244168	0.031051	0.031410	0.220572
-0.047305	0.086068	-0.037308	0.330360	0.010423

0.215386	0.032714	-0.141252	0.041486	0.124745
0.313715	0.322482	0.038545	0.012019	0.253150
-0.010218	-0.013040	0.010207	0.016534	-0.006703
-0.212106	0.368724	-0.041596	0.312938	-0.323291
-0.205711	-0.379963	-0.032795	0.048878	0.085372
0.027271	0.214865	0.021505	0.128552	0.004069

-0.207869	0.040585	-0.042785	0.051468	-0.378744
-0.302775	0.400076	0.002244	0.000701	0.014737
0.009860	0.039593	0.012669	-0.050203	-0.002019
-0.063904	0.021460	0.040131	0.388235	0.312005
-0.062351	-0.022107	0.031646	0.002844	-0.260110
0.008258	0.266550	0.006517	-0.390293	-0.012328

0.182005	0.033893	0.202504	0.042982	0.051834
0.265109	0.334111	-0.036973	-0.011529	-0.242825
-0.008632	-0.005419	0.010585	0.006871	0.009588
0.303929	-0.353684	-0.035124	0.324222	-0.273180
0.294990	0.364478	-0.027711	-0.046885	0.035981
-0.039096	0.222589	-0.030836	0.053412	0.001677

-0.140076	0.015040	-0.247151	0.019073	0.354577
-0.204039	0.148258	-0.028155	-0.008781	-0.184911
0.006643	-0.037067	0.004699	0.047000	-0.011705
-0.371300	-0.269326	0.027025	0.143870	0.210245
-0.360015	0.277543	0.021331	-0.035702	0.242953
0.047718	0.098768	0.037634	0.365389	0.011556

0.206233	0.004245	-0.247831	-0.118073	-0.091230
0.084497	0.109697	0.003024	-0.139254	-0.164545
-0.174527	-0.010857	-0.073675	-0.301972	-0.209695
0.312599	-0.067426	-0.279763	-0.035667	0.259895
-0.101568	-0.207358	0.010054	-0.223189	-0.222229
0.336165	-0.087039	-0.012086	0.280547	-0.188410

-0.217859	0.010598	0.142851	-0.294771	-0.035504
-0.089271	0.273862	0.012487	-0.216696	-0.256052

0.184363	-0.004225	-0.183927	0.117505	0.120861
-0.179922	-0.104928	0.295526	-0.089046	-0.274548
0.058549	-0.322685	-0.010627	-0.347319	-0.036857
-0.193780	-0.217299	0.006967	0.109166	-0.073296

...CONTD

0.210254	0.013148	0.043304	-0.365698	0.107789
0.086169	0.339757	0.000727	-0.012609	-0.014899
-0.177925	0.012826	-0.228175	0.356760	0.036659
-0.054887	-0.006108	-0.285195	-0.110473	0.264964
0.017742	-0.018786	0.010258	-0.020214	0.262942
-0.058720	-0.269594	0.002111	-0.331447	0.222568

-0.184092	0.010980	-0.204857	-0.305402	-0.014750
-0.075459	0.283738	-0.011977	0.207854	0.245605
0.155784	-0.001755	-0.190547	-0.048825	-0.173358
0.258188	0.100650	0.249691	-0.092259	-0.231992
-0.083955	0.309515	-0.008977	0.333156	-0.035664
0.277861	-0.225152	-0.009989	0.045363	-0.030471

0.141682	0.004872	0.250011	-0.135519	-0.100915
0.058081	0.125905	-0.009121	0.158276	0.187023
-0.119895	-0.012007	-0.084551	-0.333998	0.211563
-0.314739	0.076644	-0.192158	-0.040939	0.178544
0.102464	0.235693	0.006903	0.253694	-0.246634
-0.339118	-0.099911	0.012191	0.310301	-0.208349

-0.216901	0.000961	0.260645	-0.074558	-0.254786
0.236076	0.041352	0.001816	0.229118	0.173024
0.287205	-0.002457	0.121209	-0.190681	0.345116
0.117447	-0.188317	-0.176634	-0.099626	0.097966
-0.283647	-0.073164	0.002281	-0.140934	0.234265
0.212285	0.091531	-0.002735	0.105758	0.309984

0.229115	0.002398	-0.150224	-0.186144	-0.099165
-0.249357	0.103238	0.002826	0.356569	0.269274
-0.303376	-0.000956	0.302618	-0.074214	-0.198916
-0.067969	-0.293069	0.186589	-0.248728	-0.103484
0.163481	-0.121640	-0.002402	-0.219328	0.091037
-0.122345	0.228519	0.001576	0.041164	0.120657

-0.221112	0.002975	-0.045553	-0.230934	0.301021
0.240631	0.128080	0.000164	0.020764	0.015681
0.292776	0.002902	0.375439	0.225277	-0.060300
-0.020232	-0.017065	-0.180088	-0.308579	0.099878
0.049571	-0.007080	0.002314	-0.012772	-0.276632
-0.037102	0.283505	0.000477	-0.124942	-0.366248

0.193596	0.002485	0.215451	-0.192858	-0.041187
-0.210673	0.106962	-0.002710	-0.342021	-0.258288
-0.256341	-0.000397	0.313541	-0.030823	0.285250
0.097264	0.281110	0.157697	-0.257702	-0.087461
-0.234454	0.116680	-0.002030	0.210374	0.037971
0.175459	0.236759	-0.002260	0.017092	0.050108

-0.143996	0.001103	-0.262935	-0.085579	-0.281817
0.162131	0.047463	-0.002064	-0.260449	-0.196687

0.197285	-0.072717	0.139131	-0.210902	-0.348122
-0.119077	0.214065	-0.121379	-0.114353	0.067320
0.286125	0.088851	0.001508	0.160200	0.258809
-0.214121	0.105058	0.002759	0.116967	0.342890

CHECK OF SIMILARITY TRANSFORMATION

..CONTD

13.247914	5.390096	0.000000	0.000000	-0.000000
2.877956	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	0.000000	-0.000000
-0.000000	0.000000	-0.000000	0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

5.390096	17.858331	5.390096	0.000000	0.000000
-0.000000	2.877956	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	0.000000	0.000000	-0.000000

0.000000	5.390096	17.858331	5.390096	-0.000000
0.000000	0.000000	2.877956	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000

0.000000	0.000000	5.390096	17.858331	5.390096
-0.000000	0.000000	0.000000	2.877956	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	0.000000	-0.000000	5.390096	14.557396
-0.000000	-0.000000	0.000000	-0.000000	2.877956
-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.0
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000

2.877956	-0.000000	0.000000	-0.000000	-0.000000
10.369959	5.390096	-0.000000	0.000000	-0.000000
1.526266	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000

-0.000000	2.877956	0.000000	0.000000	-0.000000
5.390096	14.980376	5.390096	0.000000	-0.000000
-0.000000	1.526266	-0.000000	0.000000	0.000000
0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

0.000000	0.000000	2.877956	0.000000	0.000000
-0.000000	5.390096	14.980376	5.390096	-0.000000

0.000000	-0.000000	1.526266	-0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000

..CONTD

-0.000000	0.000000	0.000000	2.877956	-0.000000
0.000000	0.000000	5.390096	14.980376	5.390096
0.000000	0.000000	-0.000000	1.526266	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

-0.000000	-0.000000	0.000000	-0.000000	2.877956
-0.000000	-0.000000	-0.000000	5.390096	11.679441
0.000000	0.000000	0.000000	-0.000000	1.526266
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

-0.000000	-0.000000	0.000000	-0.000000	-0.000000
1.526266	-0.000000	0.000000	0.000000	0.000000
10.369959	5.390096	-0.000000	0.000000	0.000000
1.468651	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000

-0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	1.526266	-0.000000	0.000000	0.000000
5.390096	14.980376	5.390096	-0.000000	0.000000
-0.000000	1.468651	-0.000000	-0.000000	0.000000
0.000000	-0.000000	0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	1.526266	-0.000000	0.000000
-0.000000	5.390096	14.980376	5.390096	-0.000000
0.000000	-0.000000	1.468651	0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

-0.000000	-0.000000	0.000000	-0.000000	0.000000
0.000000	0.000000	-0.000000	1.526266	-0.000000
0.000000	-0.000000	5.390096	14.980376	5.390096
0.000000	0.000000	0.000000	1.468651	-0.000000
0.000000	-0.000000	-0.000000	0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	1.526266
0.000000	0.000000	-0.000000	5.390096	11.679441
0.000000	-0.000000	0.000000	-0.000000	1.468651
-0.000000	-0.000000	-0.000000	0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

1.468651	-0.000000	0.000000	0.000000	0.000000
10.369959	5.390096	-0.000000	0.000000	0.000000
1.453715	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000

..CONTD

0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	-0.000000	0.000000	-0.000000	0.000000
-0.000000	1.468651	-0.000000	0.000000	0.000000
5.390096	14.980376	5.390096	0.000000	0.000000
-0.000000	1.453715	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000

-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	1.468651	0.000000	0.000000
-0.000000	5.390096	14.980376	5.390096	-0.000000
-0.000000	-0.000000	1.453715	0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000

0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	0.000000	1.468651	-0.000000
0.000000	0.000000	5.390096	14.980376	5.390096
-0.000000	0.000000	0.000000	1.453715	-0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000

-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	1.468651
0.000000	0.000000	-0.000000	5.390096	11.679441
-0.000000	0.000000	0.000000	0.000000	1.453715
0.000000	-0.000000	0.000000	0.000000	0.000000

-0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
1.453715	-0.000000	-0.000000	-0.000000	-0.000000
10.369959	5.390096	-0.000000	0.000000	0.000000
1.447808	-0.000000	-0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	1.453715	-0.000000	0.000000	0.000000
5.390096	14.980376	5.390096	0.000000	0.000000
-0.000000	1.447808	-0.000000	0.000000	0.000000

-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	1.453715	0.000000	0.000000
-0.000000	5.390096	14.980376	5.390096	-0.000000
0.000000	-0.000000	1.447808	-0.000000	-0.000000

0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	1.453715	0.000000
0.000000	0.000000	5.390096	14.980376	5.390096
0.000000	-0.000000	-0.000000	1.447808	-0.000000

..CUNID

-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	1.453715
0.000000	0.000000	-0.000000	5.390096	11.679441
0.000000	0.000000	0.000000	-0.000000	1.447808

0.000000	0.000000	-0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
1.447808	-0.000000	0.000000	0.000000	0.000000
8.786357	5.390096	-0.000000	0.000000	0.000000

0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	1.447808	-0.000000	-0.000000	0.000000
5.390096	13.397379	5.390096	-0.000000	-0.000000

-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	1.447808	-0.000000	0.000000
-0.000000	5.390096	13.397379	5.390096	-0.000000

-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	1.447808	-0.000000
0.000000	-0.000000	5.390096	13.397379	5.390096

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	1.447808
0.000000	-0.000000	-0.000000	5.390096	10.096444

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

1.716131	28.641549	4.303104	24.536127	11.402647
3.611228	26.084036	23.572911	16.294853	15.798000
2.212976	17.282477	21.363514	13.177036	4.799939
9.520517	17.693099	5.385614	22.761753	6.933535
6.198199	21.015395	9.491052	19.467480	9.507551
7.972591	20.866551	12.078038	14.724958	10.004393

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.100960	-0.162936	0.121315	0.055861	-0.152813
0.141561	0.040817	-0.307993	-0.112596	0.080555
-0.141122	0.416708	-0.059566	0.142865	-0.169607
0.116069	-0.112946	0.132332	-0.059751	0.096699
-0.170125	-0.077154	-0.386019	0.105593	0.109143
-0.159045	0.042620	0.463900	0.104391	-0.152345

-0.174153	0.664220	0.114181	-0.227722	0.097098
0.244188	-0.166395	0.782626	0.286110	-0.204695
-0.243432	-0.264777	0.242822	-0.090777	-0.159652
0.109482	0.287000	0.228279	0.243578	0.166806
-0.160136	0.196049	-0.665876	-0.268317	-0.069093
-0.149703	-0.173740	0.436648	-0.066330	0.096795

-0.274452	-1.345576	-0.056530	0.461319	0.481376
0.384819	0.337082	-0.074381	-0.027190	0.019456
-0.383629	-1.312669	-0.491905	-0.450040	0.078958
-0.053660	-0.027276	0.359774	-0.493440	0.262882
0.079217	-0.018616	-1.049375	0.025501	-0.343361
0.074073	0.351949	-0.216062	-0.328840	0.479892

-0.392393	1.834917	-0.436633	-0.629086	0.107571
0.550183	-0.459667	-2.001647	-0.731756	0.523529
-0.548487	-0.293344	0.670788	-0.100570	0.610266
-0.418096	-0.734032	0.514418	0.672889	0.375864
0.612174	-0.501460	-1.500318	0.686249	-0.077236
0.572341	-0.479923	-1.669402	-0.073485	0.107255

-0.493131	-1.329545	-0.870124	0.455823	-1.201632
0.691427	0.333066	2.483916	0.909886	-0.650977
-0.689300	3.276730	-0.486036	1.123404	1.216209
-0.834567	0.912719	0.646518	-0.487562	0.472371
1.219996	0.623520	-1.885477	-0.853305	0.855934
1.140601	0.347734	-3.326889	0.820861	-1.197890

-0.102396	0.054836	0.123045	0.021043	-0.104674
0.096967	0.004399	-0.103655	-0.104477	0.081701
-0.130948	-0.140243	-0.055270	0.053819	-0.157374
0.012377	-0.077365	0.049845	-0.040928	0.013420
-0.116530	-0.008314	0.129917	0.039777	0.110549
-0.059913	0.043224	-0.156125	0.011251	-0.141359

..CONTD

-0.176630	-0.223542	0.115812	-0.085784	0.066510
0.167264	-0.017934	-0.263392	0.265482	-0.207606
-0.225881	0.089111	0.225312	-0.034196	-0.148134
0.011882	0.196588	0.085989	0.166845	0.017976
-0.109686	0.021123	0.224098	-0.101077	-0.070222
-0.056394	-0.176204	-0.146953	-0.007149	0.089819

-0.278356	0.452852	-0.057324	0.173781	0.329733
0.263592	0.036330	0.025033	-0.025232	0.019731
-0.355971	0.441777	-0.456437	-0.169533	0.073279
-0.005370	-0.018684	0.135532	-0.337994	0.028334
0.054270	-0.001991	0.353157	0.009606	-0.348208
0.027904	0.356953	0.072715	-0.035442	0.445292

-0.397973	-0.617539	-0.442828	-0.236979	0.073686
0.376862	-0.049543	0.673652	-0.678997	0.530973
-0.508943	0.098724	0.622427	-0.037886	0.566290
-0.044973	-0.502795	0.193806	0.460911	0.040518
0.419338	-0.054068	0.504927	0.258514	-0.077881
0.215607	-0.486762	0.561835	-0.007920	0.099510

-0.500145	0.447457	-0.882482	0.171711	-0.823090
0.473609	0.035898	-0.837641	0.844288	-0.660230
-0.639604	-1.102778	-0.450998	0.423195	1.128555
-0.090993	0.625193	0.243589	-0.333967	0.050927
0.835688	0.067218	0.634574	-0.321445	0.869041
0.429676	0.352697	1.119661	0.088472	-1.111553

-0.073105	-0.013704	0.087856	-0.044160	0.050242
-0.045541	-0.031813	-0.025904	-0.044152	0.058330
-0.055340	0.035047	-0.023356	-0.112938	-0.066500
-0.090680	0.037135	-0.104622	0.019646	-0.075367
0.055936	0.060136	-0.032465	-0.083474	0.078798
0.125729	0.030856	0.030016	-0.081362	-0.059738

-0.126104	0.055864	0.082699	0.180019	-0.031924
-0.080282	0.129687	0.065823	0.112193	-0.148218
-0.095460	-0.022269	0.095212	0.071761	-0.062587
-0.085188	-0.094362	-0.180469	-0.080087	-0.130009
0.052654	-0.152811	-0.056005	0.212111	-0.050253
0.118343	-0.125792	0.036724	0.051697	0.037962

-0.198730	-0.113170	-0.040903	-0.364683	-0.153266
-0.126522	-0.262720	-0.006256	-0.010663	0.014086
-0.150438	-0.110402	-0.192884	0.355765	0.030998
0.042515	0.008968	-0.284404	0.162239	-0.204889
-0.026037	0.014533	-0.088262	-0.020159	-0.248535
-0.058558	0.254339	-0.013172	0.256297	0.188187

-0.284130	0.154326	-0.316125	0.497306	-0.035367
-0.180898	0.353263	-0.163348	-0.286945	0.379082

-0.215036	-0.024571	0.263034	0.079503	0.239368
0.326023	0.241340	-0.405619	-0.221241	-0.292944
-0.201250	0.300803	-0.126183	-0.542494	-0.055125
-0.452448	-0.347529	-0.140405	0.057276	0.042046

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-0.357074	-0.111821	-0.630007	-0.360338	0.395071
-0.227344	-0.259590	0.209330	0.356798	-0.471361
-0.270305	0.275589	-0.190592	-0.888073	0.477006
0.648751	-0.300091	-0.511009	0.160307	-0.368157
-0.401091	-0.485945	-0.158563	0.674556	0.621394
-0.901665	0.251320	-0.279808	-0.639778	-0.469778

-0.058858	0.003783	0.070735	0.004797	0.092545
-0.085727	0.037289	0.007150	0.002229	0.046960
0.002793	-0.009674	0.001180	0.012267	0.003355
0.106084	0.068400	0.011369	0.036185	0.088346
0.103022	-0.070485	0.008964	0.009067	0.063674
-0.013656	0.024846	-0.010770	0.095367	0.003009

-0.101528	-0.015421	0.066583	-0.019556	-0.058802
-0.147878	-0.152011	-0.018169	-0.005665	-0.119329
0.004817	0.006147	-0.004811	-0.007794	0.003159
0.099982	-0.173808	0.019608	-0.147512	0.152392
0.096968	0.179106	0.015459	-0.023040	-0.040242
-0.012855	-0.101282	-0.010137	-0.060597	-0.001918

-0.160000	0.031239	-0.032932	0.039615	-0.291524
-0.233049	0.307943	0.001727	0.000540	0.011343
0.007589	0.030475	0.009751	-0.038642	-0.001554
-0.049188	0.016518	0.030889	0.298829	0.240154
-0.047992	-0.017016	0.024358	0.002189	-0.200210
0.006357	0.205167	0.005016	-0.300413	-0.009489

-0.228756	-0.042599	-0.254520	-0.054022	-0.065149
-0.333205	-0.419932	0.046470	0.014490	0.305198
0.010849	0.006811	-0.013304	-0.008636	-0.012051
-0.381997	0.444533	0.044146	-0.407502	0.343350
-0.370762	-0.458099	0.034828	0.058928	-0.045223
0.049139	-0.279764	0.038757	-0.067132	-0.002108

-0.287483	0.030867	-0.507235	0.039143	0.727708
-0.418755	0.304275	-0.057783	-0.018021	-0.379498
0.013634	-0.076073	0.009643	0.096459	-0.024022
-0.762030	-0.552746	0.055464	0.295268	0.431493
-0.738870	0.569611	0.043779	-0.073273	0.498621
0.097933	0.202704	0.077237	0.749900	0.023716

-0.051558	-0.001061	0.061958	0.029518	0.022808
-0.021124	-0.027424	-0.002006	0.034814	0.041136
0.043632	0.002714	0.018419	0.075493	0.052424
-0.078150	0.016850	0.069941	0.008917	-0.064974
0.025392	0.051840	-0.002514	0.055797	0.055557
-0.084041	0.021760	0.003021	-0.070137	0.047102

-0.088935	0.004326	0.058315	-0.120333	-0.014494
-0.036443	0.111797	0.005057	-0.088461	-0.104527

0.075262	-0.001725	-0.075084	-0.047968	0.049339
-0.073449	-0.042334	0.120641	-0.036351	-0.112077
0.023901	-0.131728	-0.004338	-0.141784	-0.035457
-0.079106	-0.088707	0.002844	0.044564	-0.029921

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-0.140153	-0.008764	-0.028866	0.243771	-0.071851
-0.057440	-0.226479	-0.000484	0.008405	0.009931
0.118603	-0.008550	0.152099	-0.237813	-0.024436
0.036587	0.004071	0.190108	0.073640	-0.176623
-0.011826	0.012523	-0.006838	0.013474	-0.175274
0.039142	0.179709	-0.001407	0.220939	-0.148362

-0.200380	0.011951	-0.222981	-0.332422	-0.016055
-0.082135	0.308842	-0.013037	0.226244	0.267335
0.169567	-0.001910	-0.207406	-0.053145	-0.188696
0.281032	0.109555	0.271782	-0.100422	-0.252517
-0.091383	0.336899	-0.009771	0.362632	-0.033819
0.302445	-0.245072	-0.010873	0.049376	-0.033167

-0.251822	-0.008660	-0.444361	0.240867	0.179364
-0.103231	-0.223781	0.016211	-0.281316	-0.332409
0.213097	0.021342	0.150279	0.593639	-0.376026
0.559407	-0.136225	0.341536	0.072764	-0.317339
-0.182117	-0.418915	-0.012269	-0.450908	0.438360
0.602739	0.177579	-0.021668	-0.551520	0.370314

-0.048500	0.000215	0.058282	-0.016672	-0.056972
0.052788	0.009246	0.000406	0.051232	0.038689
0.064221	-0.000549	0.027103	-0.042637	0.077170
0.026262	-0.042109	-0.039497	-0.022277	0.021906
-0.063425	-0.017478	0.000510	-0.031514	0.052383
0.047468	0.020467	-0.000611	0.023648	0.069314

-0.033656	-0.000876	0.054851	0.067966	0.036208
0.091047	-0.037695	-0.001032	-0.130193	-0.098319
0.110771	0.000349	-0.110494	0.027098	0.072630
0.024817	0.107008	-0.068129	0.090818	0.037785
-0.059691	0.044414	0.000877	0.080083	-0.033240
0.044672	-0.083439	-0.000576	-0.015030	-0.044055

-0.131830	0.001774	-0.027160	-0.137687	0.179474
0.143468	0.076363	0.000098	0.012380	0.009349
0.174558	0.001730	0.223843	0.134314	-0.035952
-0.012062	-0.010174	-0.107372	-0.183980	0.059549
0.029555	-0.004221	0.001380	-0.007615	-0.164933
-0.022121	0.169030	0.000285	-0.074492	-0.218363

-0.188478	-0.002419	-0.209755	0.187759	0.040099
0.205103	-0.104134	0.002639	0.332979	0.251459
0.249564	0.000387	-0.305251	0.030008	-0.277709
-0.094692	-0.273678	-0.153528	0.250889	0.085149
0.228256	-0.113595	0.001977	-0.204812	-0.036967
-0.170820	-0.230500	0.002201	-0.016640	-0.048783

-0.236863	0.001753	-0.417995	-0.136047	-0.448012
0.257745	0.075454	-0.003281	-0.414044	-0.312670

0.313629	-0.004319	0.221181	-0.335277	-0.553419
-0.189300	0.340605	-0.192959	-0.181739	0.107020
0.454860	0.141248	0.002493	0.254674	0.411437
-0.340394	0.167014	0.004386	0.185945	0.545103

SOLUTION OF THE DISPERSION MODELEQUATION
 USING DANCKWERTS B.C.
 SEMI-ANALYTICAL SDLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.1	0.307153	0.103866	0.026350	0.005294	0.000918
0.2	0.490677	0.264432	0.115796	0.042147	0.014024
0.3	0.617096	0.411323	0.234887	0.116031	0.054546
0.4	0.710847	0.535479	0.358254	0.214027	0.124831
0.5	0.783297	0.638762	0.474571	0.322710	0.217486
0.6	0.840724	0.724591	0.579719	0.432630	0.322561
0.7	0.887025	0.796120	0.672771	0.538010	0.431420
0.8	0.924818	0.855950	0.754144	0.635683	0.537875
0.9	0.955949	0.906168	0.824780	0.724184	0.638040
1.0	0.981776	0.948440	0.885794	0.803105	0.729803

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.0	0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.1	0.314766	0.107274	0.027323	0.005502	0.000955
0.2	0.508582	0.276936	0.121899	0.044495	0.014832
0.3	0.643210	0.433371	0.248736	0.123189	0.057994
0.4	0.743036	0.565570	0.380090	0.227526	0.132824
0.5	0.819939	0.675200	0.503551	0.342880	0.231162
0.6	0.880659	0.765949	0.614724	0.459094	0.342250
0.7	0.929427	0.841289	0.712732	0.570284	0.456903
0.8	0.969094	0.904087	0.798140	0.672600	0.568634
0.9	1.001670	0.956633	0.872051	0.765203	0.673441
1.0	1.028621	1.000746	0.935722	0.847560	0.769200

CONCENTRATIONS AT GRID POINTS

TIME	11	12	13	14	15
0.0	0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.1	0.305979	0.103258	0.026160	0.005251	0.000910
0.2	0.485250	0.259965	0.113359	0.041137	0.013657
0.3	0.605501	0.399633	0.226528	0.111296	0.052107
0.4	0.692347	0.514622	0.340748	0.201989	0.117124
0.5	0.757865	0.608014	0.445905	0.300221	0.200847
0.6	0.808714	0.684006	0.538992	0.397516	0.293840
0.7	0.848967	0.746190	0.619881	0.489113	0.388453
0.8	0.881306	0.797384	0.689505	0.572679	0.479527
0.9	0.907578	0.839763	0.749114	0.647360	0.564048
1.0	0.929111	0.875007	0.799982	0.713157	0.640549

CONCENTRATIONS AT GRID POINTS					
TIME	16	17	18	19	20
0.0	0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.1	0.305691	0.103108	0.026114	0.005241	0.000908
0.2	0.483856	0.258810	0.112726	0.040873	0.013561
0.3	0.602399	0.396476	0.224250	0.109997	0.051433
0.4	0.687215	0.508770	0.335779	0.198538	0.114898
0.5	0.750584	0.599093	0.437474	0.293526	0.195846
0.6	0.799293	0.671885	0.526635	0.386711	0.284905
0.7	0.837494	0.730897	0.603394	0.473527	0.374678
0.8	0.867910	0.779048	0.668877	0.552220	0.460329
0.9	0.892412	0.818571	0.724468	0.621864	0.539148
1.0	0.912334	0.851177	0.771529	0.682735	0.609921

CONCENTRATIONS AT GRID POINTS					
TIME	21	22	23	24	25
0.0	0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.1	0.305682	0.103103	0.026112	0.005240	0.000908
0.2	0.483780	0.258743	0.112687	0.040856	0.013554
0.3	0.602162	0.396219	0.224053	0.109880	0.051370
0.4	0.686720	0.503168	0.335237	0.198144	0.114634
0.5	0.749750	0.593007	0.436383	0.292616	0.195140
0.6	0.798061	0.670203	0.524813	0.385034	0.283463
0.7	0.835828	0.728543	0.600697	0.470956	0.372208
0.8	0.865793	0.775978	0.665205	0.548377	0.456581
0.9	0.889841	0.814768	0.719763	0.616728	0.533934
1.0	0.909318	0.846646	0.765772	0.676237	0.603122

CONCENTRATIONS AT GRID POINTS					
TIME	26	27	28	29	30
0.0	0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.1	0.305693	0.103107	0.026113	0.005240	0.000908
0.2	0.483806	0.258754	0.112691	0.040857	0.013555
0.3	0.602192	0.396230	0.224055	0.109878	0.051369
0.4	0.686738	0.508157	0.335214	0.198122	0.114617
0.5	0.749736	0.597945	0.436300	0.292536	0.195073
0.6	0.797995	0.670061	0.524628	0.384846	0.283291
0.7	0.835693	0.728291	0.600367	0.470603	0.371864
0.8	0.865574	0.775592	0.664691	0.547802	0.455994
0.9	0.889530	0.814229	0.719034	0.615881	0.533038
1.0	0.908907	0.845942	0.764803	0.675079	0.601865

APPENDIX C1

TWO DIMENSIONAL NON-HOMOGENEOUS CASE

(a) D_R and u both function of the radial position

$$\beta(R) = \frac{2 (dP/dT)}{8 + 15 R^6}$$

$$u(R) = f(R)$$

The partial differential equation describing the above problem is:

$$\frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \eta(R) \frac{\partial C}{\partial z} + \frac{\gamma}{R} \frac{\partial}{\partial R} (R \beta(R) \frac{\partial C}{\partial R})$$

$$\text{where } (R) = \frac{\text{Point velocity}}{\text{Average velocity}} = \frac{u(R)}{u_{av}}.$$

The boundary conditions are:

$$\begin{aligned} \text{(i)} \quad & \text{at } z = 0, \quad C = 1 \\ & \text{at } z = 1, \quad \frac{\partial C}{\partial z} = 0 \\ & \text{at } R = 0, \quad \frac{\partial C}{\partial R} = 0 \\ & \text{at } R = 1, \quad \frac{\partial C}{\partial R} = 0. \end{aligned}$$

$$\begin{aligned} \text{(ii)} \quad & \text{at } z = 0, \quad C_{in}(\theta) = C_{z \rightarrow 0^+} - \alpha \left(\frac{\partial C}{\partial z} \right)_{z \rightarrow 0^+} \\ & \text{at } z = 1, \quad \frac{\partial C}{\partial z} = 0 \\ & \text{at } R = 0, \quad \frac{\partial C}{\partial R} = 0 \\ & \text{at } R = 1, \quad \frac{\partial C}{\partial R} = 0. \end{aligned}$$

Semi Analytical Solution A thirty point grid was used to evaluate the concentration profile at various times. The grid spacing is as shown in Figure III-d.

(b) One D_R a function of radial position and the velocity is the overall average velocity.

The partial differential equation describing this model is:

$$\frac{\partial C}{\partial \theta} = \alpha \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} + \frac{\gamma}{R} \frac{\partial}{\partial R} (R \beta(R) \frac{\partial C}{\partial R}) .$$

The boundary conditions are the same as in case (a) and the grid spacing is also given by Figure III-d.


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C      SOLUTION OF THE DISPERSION MODEL EQUATION-TWO
C      DIMENSIONAL HOMOGENEOUS CASE
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
      REAL*8 DX,A
      DOUBLE PRECISION MATRIX(60,60),VECTOR(60,60),
1TOLERC,W(60,60),CEVR(60,60),TIME(60),CONC(15,10)
      DOUBLE PRECISION X(60),VAR(60),CI(60),C1(60)
      DOUBLE PRECISION D(60,60),VICTOR(60,60),R(15),
1SUM(15,10),CEVR1(15,10),DLV(15,10),DEVP(15,10)
C      READ THE DATA
      READ( 5,1)  N,NT
      READ(5,5)  ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 ) (CI(J),J=1,N)
      READ( 5,2 ) (C1(J),J=1,N)
      READ(5,3)  (TIME(J), J=1,NT)
      READ(5,4) DX
      DO 99 J=1,NT
      READ(5,12) (CONC(J,K),K=1,5)
99  CONTINUE
      R(1)=0.0
      READ(5,6) (R(I),I=2,6)
      NORM=2
      TOLERC=0.000
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,222)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,225)
      WRITE(6,233)
      CALL LINECT(LINES,2,2)
      WRITE(6,234) (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,2,2)
      DO 30 J=1,N
30  C1(J)=CI(J)/(DX**2)
      WRITE(6,234) (C1(J),J=1,N)
      DO 35 J=1,N

```



```

      DO 35 K=1,N
      MATRIX(J,K)=MATRIX(J,K)/(DX**2)
30  CONTINUE
      WRITE(6,220)
      WRITE(6,240)
      CALL LINECT(LINES,4,2)
      DO 31 J=1,15
      WRITE(6,241)(MATRIX(J,K),K=1,N)
31  CONTINUE
      WRITE(6,220)
      DO 62 J=15,30
      WRITE(6,241)(MATRIX(J,K),K=1,N)
62  CONTINUE
      CALL TRANS(N,IX,D,MATRIX)
      WRITE(6,255)
      CALL LINECT(LINES,1,2)
      WRITE(6,241) (D(J,J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,220)
      WRITE(6,251)
      DO 50 J=1,15
      WRITE(6,241) (MATRIX(J,K),K=1,N)
50  CONTINUE
      WRITE(6,220)
      DO 63 J=15,30
      WRITE(6,241) (MATRIX(J,K),K=1,N)
63  CONTINUE
      CALL JACOBI(N,MATRIX,VECTOR,TOLERRC,NORM)
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,5,2)
      WRITE(6,242)
      WRITE(6,232) (MATRIX(J,J),J=1,N)
      CALL LINECT(LINES,3,2)
      WRITE(6,223)
      WRITE(6,243)
      DO 32 K=1,N
      CALL LINECT(LINES,7,2)
      WRITE(6,232) (VECTOR(K,J),J=1,N)
72  WRITE(6,223)
      CALL CHECK(VECTOR,MATRIX,N,n)
      CALL LINECT(LINES,1,2)
      WRITE(6,223)
      WRITE(6,244)
      DO 33 J=1,N
      CALL LINECT(LINES,7,2)
      WRITE(6,232) (W(J,K),K=1,N)
77  WRITE(6,223)
      CALCULATE THE TRANSPOSE OF THE MATRIX OF
      THE EIGENVECTORS

```



```

      DO 40 I=1,N
      DO 40 J=1,N
      VECTOR(I,J)=VECTOR(J,I)
40 CONTINUE
C      A=(D(-1)*A(*)*D)
C      A(*)=THE ORIGINAL COEFFICIENT MATRIX
C      D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C      OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C      A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C      COEFFICIENT MATRIX A(*)
C      Q=THE MATRIX OF EIGENVECTORS OF A
C      CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C      COEFFICIENT MATRIX
      DO 38 I=1,N
      DO 38 J=1,N
      VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,6,2)
      WRITE(6,256)
      WRITE(6,232) (MATRIX(J,J),J=1,N)
      CALL LINECT(LINES,3,2)
      WRITE(6,223)
      WRITE(6,257)
      DO 39 K=1,N
      CALL LINECT(LINES,7,2)
      WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
C      (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
C      QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
C      D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
C      CALCULATE THE PRODUCT (QT*D(-1))
      DO 41 I=1,N
      DO 41 J=1,N
      VECTOR(I,J)=VECTOR(I,J)/D(J,J)
41 CONTINUE
      CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
      ICEVF,VECTOR)
      WRITE(6,220)
      WRITE(6,225)
      WRITE(6,245)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,248)
      DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVF(J,K),K=1,5)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,249)

```



```

      DO 35 J=1,NT
35  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=6,10 )
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,254)
      DO 45 J=1,NT
45  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=11,15)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,260)
      DO 46 J=1,NT
46  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=16,20)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,265)
      DO 60 J=1,NT
60  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=21,25)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,266)
      DO 61 J=1,NT
61  WRITE(6,251)  TIME(J),  (CEVR(J,K),K=26,30)
      SUM1=0.0
      DO 9 I=1,6
      SUM1=SUM1+R(I)
9  CONTINUE
      DO 8 J=1,NT
      DO 8 K=1,5
      SUM(J,K)=R(1)*CEVR(J,K)+R(2)*CEVR(J,K+5)
      1+R(3)*CEVR(J,K+10)+R(4)*CEVR(J,K+15)
      2+R(5)*CEVR(J,K+20)+R(5)*CEVR(J,K+25)
      CEVR1(J,K)=SUM(J,K)/SUM1
8  CONTINUE
      DO 10 J=1,NT
      DO 10 K=1,5
      DEV(J,K)=CEVR1(J,K)-CONC(J,K)
10  CONTINUE
      A=100.0
      DO 16 K=1,5
      DEVP(1,K)=0.0
16  CONTINUE
      DO 11 J=2,NT
      DO 11 K=1,5
      DEVP(J,K)=(DEV(J,K)/CEVR1(J,K))*A
11  CONTINUE
      WRITE(6,223)
      WRITE(6,270)
      WRITE(6,223)
      WRITE(6,246)
      DO 7 J=1,NT

```



```

      WRITE(6,251)  TIME(J),  (CONC(J,K),K=1,5)
7  CONTINUE
      WRITE(6,225)
      WRITE(6,271)
      WRITE(6,248)
      DO 15 J=1,NT
      WRITE(6,251)  TIME(J),  (CEVR1(J,K),K=1,5)
15 CONTINUE
      WRITE(6,227)
      WRITE(6,272)
      WRITE(6,223)
      WRITE(6,243)
      DO 13 J=1,NT
      WRITE(6,251)  TIME(J),  (OLV(J,K),K=1,5)
13 CONTINUE
      WRITE(6,273)
      WRITE(6,223)
      WRITE(6,243)
      DO 14 J=1,NT
      WRITE(6,251)  TIME(J),  (OEVP(J,K),K=1,5)
14 CONTINUE

```

FORMAT STATEMENTS

```

1  FORMAT(1X,2I4)
2  FORMAT(10F3.5)
3  FORMAT(11F7.3)
4  FORMAT(1X,F16.8)
5  FORMAT(10F3.5)
6  FORMAT(1X,F13.8,4F14.8)
12 FORMAT(5F15.6)
227 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,23H CONCENTRATION PROFILES-TWO-,
      111HDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,19HUSING ORDINARY B.C.)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,25H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,12H COEFFICIENT MATRIX)
241 FORMAT(1H,5X,10F6.2)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
246 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 8X, 2H 2, 4X,
      12H 3, 8X, 2H 4, 8X, 2H 5)

```



```

247 FORMAT(1H,15X,5H TIME,9X,2H 5,0X,2H 7,0X,2H 3,
18X,2H 9,8X,2H10)
251 FORMAT(1H,15X,F5.1,2X,5F17.6)
253 FORMAT(1H,10X,13HGRID SPACING=,F11.6)
255 FORMAT(1H,10X,9HMATRIX(D)/10X,
119H(DIAGONAL ELEMENTS))
256 FORMAT(1H,20X,17H EIGENVALUES OF THE/20X,
127HORIGINAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,27H EIGENVECTORS OF THE/20X,
127HORIGINAL COEFFICIENT MATRIX)
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,
18X,2H14,8X,2H15)
260 FORMAT(1H,15X,5H TIME,4X,2H16,8X,2H17,8X,2H18,
18X,2H19,8X,2H20)
261 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX/
120X,25H(CONVERTED INTO SYMMETRIC))
265 FORMAT(1H,15X,5H TIME,4X,2H21,8X,2H22,6X,2H23,
18X,2H24,8X,2H25)
266 FORMAT(1H,15X,5H TIME,4X,2H26,8X,2H27,8X,2H28,
18X,2H29,8X,2H30)
270 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
111HDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)
271 FORMAT(1H,10X,16HWEIGHTED AVERAGE/
110X,32HTWO DIMENSIONAL HOMOGENEOUS CASE)
272 FORMAT(1H,20X,18HABSOLUTE DEVIATION)
273 FORMAT(1H,20X,17HPERCENT DEVIATION)
STOP
END

```


SUBROUTINE TRANS(N,DX,D,MATRIX)

THIS SUBROUTINE CONVERTS THE ORIGINAL COEFFICIENT
MATRIX TO THE REAL SYMMETRIC FORM USING
SIMILARITY TRANSFORMATION

INPUT DATA

DX= THE GRID SPACING

N= THE NUMBER OF GRID POINTS

D=THE DIAGONAL MATRIX ,WITH DIAGONAL ENTERIES

HAVING ALTERNATE SIGNS I.E. $D(I,I)=(-1)**(I)(D(I,I))$

USED FOR SIMILARITY TRANSFORMATION

MATRIX= THE ORIGINAL COEFFICIENT MATRIX (DIAGONALLY
DOMINANT & UNSYMMETRIC), DESTROYED DURING
COMPUTATION AND THE RESULTANT MATRIX IS SYMMETRIC
AND DIAGONALLY DOMANANT.

REAL*8 DX,ALPHA,BETA,A1,A2,A3

DOUBLE PRECISION D(60,60),MATRIX(60,60)

ALPHA=0.2

BETA=DX/2.0

D(1,1)=1.0

CALCULATE THE DIAGONAL ELEMENTS OF MATRIX D.

DO 100 I=1,4

II=I+1

$D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))$

100 CONTINUE

A1=2.0

$D(6,6)=1.0/(2.0*DSQRT(A1))$

DO 101 I=6,9

II=I+1

$D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))$

101 CONTINUE

$D(11,11)=0.25$

DO 102 I=11,14

II=I+1

$D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))$

102 CONTINUE

A2=6.0

$D(16,16)=1.0/(2.0*DSQRT(A2))$

DO 103 I=16,19

II=I+1

$D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))$

103 CONTINUE

$D(21,21)=1.0/(4.0*DSQRT(A1))$

DO 104 I=21,24

II=I+1

$D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))$

104 CONTINUE

A3=10.0

$D(26,26)=1.0/(2.0*DSQRT(A3))$


```

      DO 105 I=26,29
      II=I+1
      D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))
105  CONTINUE
      DO 106 I=1,30,2
      D(I,I)=-D(I,I)
106  CONTINUE
C
C      CALCULATE THE COEFFICIENT MATRIX CONVERTED INTO
C      THE SYMMETRIC ONE
C
      DO 107 I=1,N
      DO 107 J=1,N
      MATRIX(I,J)=(MATRIX(I,J)*D(J,J))/(D(I,I))
107  CONTINUE
      RETURN
      END

```


INITIAL CONDITION VECTOR

BOUNDARY CONDITION VECTOR

ORIGINAL COEFFICIENT MATRIX

(CONVERTED INTO SYMMETRIC)

EIGENVALUES

2.332570	30.322215	25.993119	27.490049	3.097461
5.722366	20.220725	14.671200	25.333712	4.553756
11.478993	20.984629	23.466363	13.295381	23.090390
17.318164	7.245605	17.611631	8.576634	11.968310
6.472274	22.012512	6.482362	10.067944	21.243858
15.211947	0.952124	15.844790	11.772170	11.839111

EIGENVECTORS

0.021906	0.264749	-0.447226	-0.097729	0.045908
0.042265	-0.492238	0.392662	-0.293725	-0.052520
-0.123692	0.158284	0.081349	0.151188	0.165090
0.181632	-0.120263	0.125974	0.271437	0.144076
0.070078	0.262763	0.091441	0.137426	-0.023717
-0.174111	-0.138289	0.045532	-0.053497	0.116677

-0.038083	0.448089	-0.293465	-0.165746	-0.083220
-0.050137	0.294007	-0.462342	-0.158040	0.107901
0.351152	0.139286	0.137981	-0.028861	0.145262
-0.034684	0.142119	0.093306	-0.129541	-0.170572
-0.125075	0.126459	-0.107511	0.120936	-0.046712
0.033210	0.163679	0.042687	0.010248	-0.022313

0.048037	0.426710	0.101023	-0.183370	0.104980
0.015964	0.474251	0.156562	-0.175818	-0.136091
-0.442791	-0.035734	0.152673	-0.145709	-0.037275
-0.175031	-0.043159	-0.023901	0.163443	0.057772
0.157235	0.117792	0.034594	-0.031028	-0.053894
0.167826	-0.055441	-0.010979	0.051376	-0.112424

-0.043005	0.323398	0.482347	-0.145237	-0.107092
0.030077	-0.134506	0.276991	-0.139239	0.138818
0.451643	-0.170740	0.120937	0.056722	-0.178054
0.063122	-0.045091	-0.114392	-0.166772	0.102326
-0.158788	0.073299	0.063320	-0.143253	-0.042677
-0.065299	-0.098037	-0.052327	-0.019988	0.043877

0.042803	0.170460	0.323359	-0.062935	0.082188
-0.052582	-0.438750	-0.484395	-0.060332	-0.115576
-0.376033	-0.114478	0.052409	0.134393	-0.110374
0.161974	0.140855	-0.076716	0.138876	-0.178975
0.131184	0.040427	-0.117050	-0.099408	-0.013488
-0.155396	0.171254	-0.035260	-0.047638	0.103893

-0.059423	0.158868	-0.264978	0.048168	-0.115696
-0.110663	-0.201437	0.231377	0.119995	-0.118895
-0.114679	-0.293746	-0.102521	-0.302057	-0.081393
-0.082507	0.239617	-0.269528	-0.035149	-0.070952
-0.001690	-0.169600	-0.233903	-0.274547	0.031254
0.223110	0.177126	-0.137264	0.151730	-0.296574

..CONTD

0.107730	0.266038	-0.233134	0.081686	0.211563
0.141864	0.055741	-0.273932	0.203509	-0.215535
0.207969	-0.176371	-0.275629	0.057723	-0.071615
-0.017093	-0.283891	-0.237150	0.063737	0.084184
0.163775	-0.270637	0.275927	-0.241550	0.137792
-0.042657	-0.200614	-0.120746	-0.028950	0.056745

-0.135880	0.204313	0.059361	0.040360	-0.265864
-0.043028	0.260380	0.092353	0.225145	0.271838
-0.262380	0.049790	-0.304933	0.291019	0.018365
0.086285	0.006160	0.060373	-0.080554	-0.023755
-0.202281	-0.229410	-0.091038	0.062020	0.152431
-0.214901	0.070263	0.031019	-0.145510	0.205634

0.138630	0.233097	0.285801	0.071557	0.272239
-0.085049	-0.100411	0.164093	0.173320	-0.277277
0.267650	0.218620	-0.241517	-0.113329	0.087742
-0.033566	0.170018	0.240733	0.032253	-0.050272
0.201941	-0.237142	-0.170239	0.296111	0.120732
0.033706	0.125590	0.143026	0.056691	-0.111244

-0.115424	0.101004	0.191595	0.031602	-0.226661
0.143727	-0.250091	-0.287078	0.077268	0.230847
-0.222825	0.146654	-0.104657	-0.269366	0.053812
-0.079797	-0.297373	0.194930	-0.263513	0.038255
-0.165565	-0.102770	0.294741	0.198510	0.052321
0.198844	-0.210587	0.090238	0.134644	-0.264438

0.084085	0.066306	-0.112839	0.139591	0.114285
0.169674	-0.124125	0.093502	0.146439	-0.013097
-0.048817	-0.247344	0.017875	0.033248	-0.320259
-0.352326	-0.026369	0.264086	-0.138660	-0.270936
-0.103204	0.156306	0.232323	0.030177	-0.114963
0.272102	0.215961	0.194179	-0.213688	0.290287

-0.152446	0.113297	-0.099275	0.321528	-0.207197
-0.200251	0.023732	-0.116623	0.248352	0.023725
0.083497	-0.217592	0.030286	-0.006377	-0.281750
0.067397	0.031170	0.232258	0.251373	0.331170
0.184525	0.265080	-0.276130	0.026537	-0.194903
-0.052062	-0.255672	0.170899	0.040326	-0.055337

0.192289	0.126838	0.025498	0.355691	0.261360
0.068091	0.119583	0.030568	0.274740	-0.024887
-0.111853	0.056030	0.034460	-0.031994	-0.072383
0.330746	-0.010495	-0.050748	-0.317645	-0.112074
-0.243272	0.203040	0.096577	-0.006827	-0.215718
-0.262140	0.046696	-0.043849	0.205926	-0.279922

-0.136134	0.003364	0.121707	0.281691	-0.266640
0.120266	-0.046817	0.089819	0.217597	0.030445

0.111088	0.215815	0.235402	0.312430	0.34542
-0.122328	-0.013779	-0.24474	0.323426	-0.153272
0.252514	0.282123	0.150245	-0.242519	-0.177847
0.172135	0.153493	-0.204555	-0.089218	0.108974

..CONFID

0.153404	0.244506	0.251573	0.122033	0.222079
-0.210458	-0.110408	-0.122266	0.294270	-0.025321
-0.095013	0.178312	0.211450	0.229555	0.231493
-0.314147	0.030753	-0.190708	-0.269369	0.346697
-0.212821	0.105595	-0.282475	-0.021774	-0.074012
0.242634	-0.267065	-0.140454	-0.190615	0.259142

-0.102240	0.224574	-0.041498	0.199061	-0.055864
-0.207753	-0.045652	0.035246	-0.095920	-0.114924
-0.017889	0.162145	0.157275	0.292195	-0.336219
-0.369899	-0.231879	-0.129013	-0.145578	-0.293499
0.063308	-0.076441	-0.113866	0.265600	0.147779
-0.178394	-0.141527	-0.237873	0.261710	-0.142101

0.135631	0.241675	-0.035501	0.337580	0.101283
0.245966	0.013775	-0.042902	-0.152738	0.203378
0.032470	0.142845	0.265697	-0.055907	-0.295768
0.070773	0.274473	-0.113559	0.263914	0.347603
-0.125018	-0.129612	0.135533	0.233648	0.238736
0.034119	0.167667	-0.209193	-0.050103	0.127405

-0.235423	0.046124	0.009394	0.373459	-0.127764
-0.083446	0.243238	0.014532	-0.180081	-0.262845
-0.041041	-0.030656	0.294994	-0.281484	0.076050
0.356381	-0.032985	0.029125	-0.332874	-0.113022
0.159745	-0.143467	-0.047920	-0.060053	0.264089
0.171375	-0.056866	0.053319	-0.252065	0.136697

0.240134	0.225513	0.044777	0.295764	0.131356
-0.147134	-0.017139	0.025593	-0.142614	0.268267
0.041973	-0.174896	0.233591	0.100739	0.362708
-0.138927	-0.164479	0.133237	0.339578	-0.208038
-0.155076	-0.113523	-0.077112	-0.236471	0.209132
-0.066993	-0.100447	0.255469	0.048288	-0.053454

-0.200050	0.215013	0.020037	0.123130	-0.106575
0.257972	-0.040706	-0.044936	-0.061782	-0.223486
-0.035023	-0.117207	0.101185	0.280432	0.243069
-0.329342	0.237771	0.093348	-0.262804	0.324347
0.138709	-0.049176	0.137476	-0.191974	0.090601
-0.159066	0.175648	0.171339	0.233239	-0.126341

0.118769	0.006913	-0.011458	0.133287	-0.037509
0.239637	-0.012664	0.010691	-0.190145	0.101751
-0.024377	0.328775	-0.139215	-0.254702	-0.182928
-0.201295	0.205393	-0.306602	-0.079110	-0.150745
0.144319	-0.081783	-0.073126	-0.235168	-0.162415
-0.270062	-0.293762	0.274324	-0.301833	-0.095477

-0.215117	0.011555	-0.010109	0.183645	0.080002
-0.283500	0.008413	-0.011809	-0.337733	-0.184502

-0.002485	-0.0035927	-0.236112	-0.043477	-0.180944
-0.002425	-0.0035171	-0.076215	0.183463	-0.189102
-0.262445	-0.0025950	-0.004007	-0.206893	-0.275440
0.077780	-0.747767	0.241366	0.057710	0.018391

..CONTD

0.271596	0.012782	0.002616	0.203158	-0.085707
0.095190	0.012192	0.003089	-0.373613	0.232795
-0.011415	-0.078051	-0.261224	0.249261	0.041315
0.193883	0.082533	0.013563	-0.181038	-0.064114
0.332438	-0.006155	-0.035927	0.053160	-0.304701
0.356533	-0.117327	-0.061990	0.290812	0.091797

-0.277094	0.010123	0.012423	0.160843	0.087490
0.169702	-0.004748	0.007135	-0.295890	-0.237559
0.011677	-0.362833	-0.206397	-0.097147	0.197265
-0.076490	0.145481	0.093427	0.184784	-0.113202
-0.340595	-0.076124	-0.047972	0.253670	-0.241302
-0.138970	-0.208180	-0.295924	-0.113333	-0.035894

0.230781	0.004336	0.008323	0.069702	-0.072856
-0.207155	-0.011281	-0.012422	-0.128185	0.107900
-0.009703	-0.243164	-0.087638	-0.230710	0.132203
-0.179369	-0.294698	0.062615	-0.153955	0.198123
0.284509	-0.032068	0.089139	0.170015	-0.104531
-0.329969	0.364373	-0.108329	-0.269125	-0.084822

-0.132738	0.001029	-0.001735	0.025560	0.141670
-0.267804	-0.001314	0.001536	-0.079480	0.109407
-0.000822	0.134204	-0.149498	-0.277395	-0.043210
-0.047427	0.220653	0.327171	-0.018627	-0.037941
0.052873	0.103562	0.284792	-0.252560	0.181595
-0.147752	-0.117340	-0.306711	0.337376	0.350943

0.240737	0.001748	-0.001525	0.043353	-0.256834
0.316967	0.000363	-0.001301	-0.134826	-0.198319
0.001363	0.113166	-0.253541	0.053094	-0.038031
0.009169	-0.261159	0.287853	0.033821	0.044702
-0.111026	0.328446	-0.335472	-0.222211	0.307977
0.028223	0.133350	-0.269351	-0.064469	-0.068740

-0.303654	0.001831	0.000398	0.047971	0.323943
-0.107338	0.001445	0.000591	-0.149131	0.250091
-0.001633	-0.033307	-0.280491	0.267740	0.009726
0.045716	0.088405	-0.273909	-0.042743	-0.014923
0.134841	0.363367	0.112353	0.057047	0.240719
0.142349	-0.047000	0.053288	-0.325664	-0.346347

0.304766	0.001320	0.001373	0.037992	-0.030454
-0.184955	-0.000714	0.001084	-0.118110	-0.255057
0.001735	-0.144002	-0.222152	-0.104261	0.046560
-0.017835	0.150418	-0.383860	0.043677	-0.026820
-0.132243	0.207790	0.200385	0.272394	0.269865
-0.055414	-0.082173	0.330817	0.126587	0.135044

-0.267931	0.000669	0.001299	0.016402	0.275137
0.332207	-0.001704	-0.001865	-0.051170	0.212321

-0.001556	-0.007072	-0.008202	-0.007724	0.001215
-0.042661	-0.233371	-0.233567	-0.230601	0.046592
0.107012	0.107211	-0.056277	0.102500	0.016939
-0.131724	0.100611	0.021761	0.300894	0.021070

CHECK UP SIMILARITY TRANSFORMATION

..CONTD

19.665433	5.390096	0.000000	-0.000000	-0.000000
2.673878	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

5.390096	19.665433	5.390096	0.000000	0.000000
0.000000	2.673878	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	5.390096	19.665433	5.390096	0.000000
0.000000	0.000000	2.673878	0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000

-0.000000	0.000000	5.390096	19.665433	5.390096
-0.000000	0.000000	0.000000	2.673878	-0.000000
0.000000	0.000000	0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	0.000000	0.000000	5.390096	19.665433
-0.000000	-0.000000	0.000000	-0.000000	2.673878
0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	0.000000	-0.000000	-0.000000

2.673878	0.000000	0.000000	-0.000000	-0.000000
19.665433	5.390096	-0.000000	0.000000	0.000000
2.004544	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	2.673878	0.000000	0.000000	-0.000000
5.390096	19.665433	5.390096	0.000000	0.000000
-0.000000	2.004544	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000

0.000000	-0.000000	2.673878	0.000000	0.000000
-0.000000	0.000000	19.665433	5.390096	-0.000000

0.000000	-0.000000	2.004544	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	0.000000	-0.000000

..CONTD

-0.000000	0.000000	0.000000	2.673878	-0.000000
0.000000	0.000000	5.390096	15.834427	5.390096
-0.000000	-0.000000	0.000000	2.004544	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	0.000000	0.000000	-0.000000	2.673878
0.000000	0.000000	-0.000000	5.390096	12.53517
-0.000000	-0.000000	0.000000	-0.000000	2.004544
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	-0.000000	0.000000	0.000000
2.004544	-0.000000	0.000000	-0.000000	-0.000000
15.8345094	5.390096	-0.000000	0.000000	-0.000000
1.899704	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	2.004544	-0.000000	-0.000000	-0.000000
5.390096	15.8345094	5.390096	0.000000	0.000000
0.000000	1.899704	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000

0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	2.004544	0.000000	-0.000000
-0.000000	5.390096	15.8345094	5.390096	-0.000000
0.000000	-0.000000	1.899704	0.000000	-0.000000
0.000000	0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	0.000000	0.000000	-0.000000

0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	0.000000	2.004544	-0.000000
0.000000	0.000000	5.390096	15.8345094	5.390096
-0.000000	-0.000000	0.000000	1.899704	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	2.004544
-0.000000	0.000000	-0.000000	5.390096	12.544159
-0.000000	-0.000000	0.000000	0.000000	1.899704
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	0.000000

0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000

1.899774	5.390096	0.000000	-0.000000	-0.000000
15.615148	0.000000	-0.000000	0.000000	0.000000
1.699413	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	0.000000

..CONTD

-0.000000	-0.000000	0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	1.899774	-0.000000	-0.000000	0.000000
5.390096	15.615148	5.390096	0.000000	0.000000
-0.000000	1.699413	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000

-0.000000	-0.000000	0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	1.899774	0.000000	0.000000
-0.000000	5.390096	15.615148	5.390096	-0.000000
0.000000	-0.000000	1.699413	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000

-0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	-0.000000	0.000000	-0.000000	0.000000
-0.000000	0.000000	0.000000	1.899774	0.000000
0.000000	0.000000	5.390096	15.615148	5.390096
-0.000000	-0.000000	0.000000	1.699413	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000

0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	1.899774
0.000000	0.000000	-0.000000	5.390096	12.314213
-0.000000	0.000000	0.000000	-0.000000	1.699413
-0.000000	-0.000000	-0.000000	0.000000	-0.000000

0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
1.699413	-0.000000	0.000000	-0.000000	-0.000000
14.937412	5.390096	-0.000000	0.000000	0.000000
1.217786	-0.000000	-0.000000	-0.000000	-0.000000

0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	1.699413	-0.000000	-0.000000	0.000000
5.390096	14.937412	5.390096	0.000000	0.000000
0.000000	1.217786	-0.000000	-0.000000	0.000000

0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	1.699413	0.000000	5.390096
-0.000000	5.390096	14.937412	5.390096	-0.000000
-0.000000	0.000000	1.217786	-0.000000	0.000000

0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	0.000000

-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	1.099413	-0.000000
-0.000000	0.000000	5.390096	14.937412	5.390096
-0.000000	-0.000000	0.000000	1.217766	-0.000000

..CONTD

0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	1.099413
0.000000	0.000000	-0.000000	5.390096	11.836477
-0.000000	-0.000000	0.000000	-0.000000	1.217766

-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
1.217766	0.000000	-0.000000	-0.000000	-0.000000
13.191638	5.390096	-0.000000	0.000000	0.000000

-0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	1.217766	0.000000	-0.000000	-0.000000
5.390096	13.191638	5.390096	0.000000	0.000000

-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	-0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	1.217766	0.000000	0.000000
-0.000000	5.390096	13.191638	5.390096	-0.000000

0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	1.217766	-0.000000
0.000000	0.000000	5.390096	13.191638	5.390096

0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	1.217766
0.000000	0.000000	-0.000000	5.390096	9.893729

EIGENVALUES OF THE ORIGINAL COEFFICIENT MATRIX

2.342672	40.392012	25.993112	27.490049	3.997451
5.722365	20.220725	14.871000	25.393712	4.553756
11.479993	20.054509	23.466963	13.295381	23.990890
17.318164	7.945805	17.611531	2.576634	11.962310
6.470374	22.212612	6.469352	19.067944	21.243856
15.211947	9.962124	16.844790	11.072170	11.839111

EIGENVECTORS OF THE ORIGINAL COEFFICIENT MATRIX

-0.021006	-0.214745	0.447206	0.097729	-0.045908
-0.042365	-0.492736	-0.390602	0.043725	0.059520
0.193690	-0.158234	-0.081349	-0.151138	-0.165090
-0.181632	0.120066	-0.105974	-0.071437	-0.144076
-0.070078	-0.062763	-0.091441	-0.137426	0.023717
0.174111	0.130259	-0.048532	0.053407	-0.116677

-0.062186	0.733154	-0.642489	-0.270646	-0.135003
-0.081869	0.153504	-0.754958	-0.259534	0.176192
0.573310	0.227447	0.225308	-0.047127	0.237199
-0.056635	0.032066	0.152359	-0.211527	-0.273526
-0.205868	0.173337	-0.175554	0.197477	-0.079542
0.054229	0.267262	0.069704	0.016733	-0.035435

-0.128034	-1.224909	-0.269365	0.438932	-0.274914
-0.045232	-1.063002	-0.417450	0.468795	0.362667
1.180640	0.033773	-0.407091	0.388513	0.094388
0.468616	0.128410	0.063727	-0.425797	-0.154042
-0.419513	-0.314376	-0.092001	0.032731	0.143700
-0.447486	0.147826	0.023275	-0.136935	0.290764

-0.213241	1.718014	2.100090	-0.632347	-0.466269
0.130052	-0.803713	1.205989	-0.606231	0.604400
1.964426	-0.743359	0.526549	0.246562	-0.775231
0.296536	-0.270670	-0.499053	-0.726107	0.445515
-0.691260	0.406210	0.297459	-0.645499	-0.185811
-0.084295	-0.426021	-0.227328	-0.037010	0.191035

-0.240021	-1.211424	-2.293913	0.447445	-0.533939
0.373831	0.119739	3.443800	0.428930	0.621683
2.673401	0.913877	-0.372603	-0.458952	0.848636
-1.151551	-1.768279	0.543409	-0.087340	1.272419
-0.032642	-0.207414	0.832164	0.706706	0.131437
1.104714	-1.212351	0.249257	0.338667	-0.739625

-0.021006	0.055455	-0.093670	0.017027	-0.041253
-0.042372	-0.102345	-0.081732	0.042419	0.042029
-0.040539	-0.071071	-0.057451	-0.106777	-0.023773
-0.031673	0.044178	-0.093278	-0.012425	-0.025082
-0.032416	-0.056411	-0.052685	-0.097055	0.023723
0.073869	0.062514	-0.043523	0.033373	-0.104633

..CONTD

-0.062185	-0.153865	0.134572	-0.047151	-0.122123
-0.031938	-0.022176	0.158122	-0.117471	0.124413
-0.120248	0.102954	0.159101	-0.033320	0.041338
-0.004357	0.163247	0.136390	-0.036820	-0.048594
-0.094538	0.188220	-0.154279	0.139437	-0.079533
-0.024623	0.120296	0.069598	0.016653	-0.032755

-0.123084	0.277407	0.051423	0.065169	-0.251535
-0.045269	0.264746	0.087520	0.212213	0.255223
-0.247308	0.043160	-0.287417	0.274302	0.017310
0.031329	0.090937	0.057377	-0.075927	-0.027103
-0.190662	-0.202211	-0.085309	0.058458	0.143676
-0.202557	-0.066388	0.029237	-0.137152	0.269227

-0.213385	-0.358761	-0.439877	-0.110134	-0.419004
-0.130900	0.168306	-0.252556	-0.274453	0.425757
-0.411455	-0.356493	0.371720	0.174424	-0.135043
0.051662	-0.261572	-0.447463	-0.126596	0.077374
-0.310808	0.264394	0.262092	-0.455745	-0.185818
-0.128832	-0.103206	-0.227828	-0.087254	0.171216

-0.290108	0.253244	0.481516	0.077914	-0.569695
0.372782	-0.653409	-0.721486	0.194198	0.580165
-0.550004	0.368319	-0.263023	-0.676972	0.147806
-0.200545	-0.747352	0.489899	-0.172187	0.221803
-0.416090	-0.258281	0.740744	0.498896	0.131493
0.490724	-0.551866	0.249406	0.338386	-0.664585

-0.021317	-0.016495	0.023204	-0.047383	-0.028560
-0.042410	0.031025	-0.024621	-0.036602	0.003274
0.012202	0.061324	-0.004468	-0.008310	0.080049
0.088064	0.006389	-0.065008	0.034600	0.069970
0.025796	-0.039069	-0.058069	-0.007543	0.023735
-0.068012	-0.093972	-0.043535	0.053411	-0.072557

-0.062280	0.066942	-0.040518	0.131230	-0.084566
-0.081976	0.090686	-0.047599	0.101363	0.000683
0.036110	-0.040809	0.012361	-0.002603	-0.114994
0.027534	0.012722	0.094795	0.102596	0.135165
0.077353	0.103101	-0.112701	0.010831	-0.079581
-0.021249	-0.104361	0.069751	0.016663	-0.022585

-0.120199	-0.003632	-0.016393	-0.237052	-0.174185
-0.045373	-0.079027	-0.026370	-0.183108	0.019916
0.074412	-0.037376	-0.022300	0.021323	-0.043240
-0.224228	-0.056304	0.039319	0.211294	0.074592
0.162130	-0.105432	-0.064364	0.004553	0.143767
0.174710	-0.057778	0.020224	-0.137239	0.186555

-0.213304	0.109027	0.130449	0.065552	-0.297182
0.180079	-0.098731	-0.075931	0.215803	0.033132

0.124847	0.000000	0.000000	0.000000	0.000000
-0.144001	-0.000000	-0.000000	-0.000000	-0.000000
0.274712	0.000000	0.000000	0.000000	0.000000
0.111219	0.000000	0.000000	0.000000	0.000000

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-0.292872	-0.000000	-0.000000	-0.000000	-0.000000
0.373001	0.000000	0.000000	0.000000	0.000000
0.168839	-0.000000	-0.000000	-0.000000	-0.000000
0.558262	-0.000000	0.000000	0.000000	-0.000000
0.278204	-0.000000	0.000000	0.000000	0.000000
-0.431147	0.000000	0.000000	0.000000	-0.000000

-0.021008	0.000000	-0.000000	0.000000	-0.000000
-0.042430	-0.000000	0.000000	-0.000000	-0.000000
-0.003651	0.000000	0.000000	0.000000	-0.000000
-0.075487	-0.000000	-0.000000	-0.000000	-0.000000
0.013940	-0.000000	-0.000000	0.000000	0.000000
-0.036407	-0.000000	-0.000000	0.000000	-0.000000

-0.052193	-0.000000	0.000000	-0.000000	-0.000000
-0.081955	-0.000000	0.000000	0.000000	-0.000000
-0.010820	-0.000000	-0.000000	0.000000	-0.000000
-0.023555	-0.000000	0.000000	-0.000000	-0.000000
0.041661	0.000000	-0.000000	-0.000000	-0.000000
-0.011370	-0.000000	0.000000	0.000000	-0.000000

-0.128106	0.000000	0.000000	0.000000	-0.000000
-0.045407	0.000000	0.000000	-0.000000	-0.000000
-0.022332	-0.000000	0.000000	-0.000000	0.000000
0.103925	-0.000000	0.000000	-0.000000	-0.000000
0.086925	-0.000000	-0.000000	-0.000000	0.000000
0.003526	-0.000000	0.000000	-0.000000	0.000000

-0.213423	-0.000000	-0.000000	-0.000000	-0.000000
0.130725	0.000000	-0.000000	0.000000	-0.000000
-0.037235	0.000000	-0.000000	-0.000000	-0.000000
0.123452	0.000000	-0.000000	-0.000000	0.000000
0.146677	0.000000	0.000000	0.000000	-0.000000
0.059528	0.000000	-0.000000	-0.000000	0.000000

-0.292261	0.000000	0.000000	0.000000	-0.000000
0.373712	-0.000000	-0.000000	-0.000000	-0.000000
-0.050815	-0.000000	0.000000	0.000000	0.000000
-0.478568	0.000000	0.000000	-0.000000	0.000000
0.201252	-0.000000	0.000000	-0.000000	0.000000
-0.230742	0.000000	0.000000	0.000000	-0.000000

-0.020933	-0.000000	0.000000	-0.000000	0.000000
-0.042351	0.000000	-0.000000	0.000000	-0.000000
0.000362	-0.000000	0.000000	0.000000	0.000000
0.035575	-0.000000	0.000000	0.000000	0.000000
-0.025506	0.000000	0.000000	0.000000	0.000000
0.085631	0.000000	-0.000000	0.000000	0.000000

-0.062135	0.000000	-0.000000	0.000000	0.000000
-0.081865	0.000000	-0.000000	-0.000000	-0.000000

0.002584	0.001347	-0.004138	0.014276	-0.046445
0.011040	-0.001178	-0.021992	0.041401	0.064571
-0.075737	-0.009790	0.027123	-0.069736	-0.079487
0.030428	0.003367	0.069654	0.015554	0.005307

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-0.127933	-0.006929	-0.001233	-0.045733	0.040415
-0.045327	-0.005745	-0.001380	0.176054	-0.103695
0.005374	0.039337	0.123025	-0.117459	-0.010469
-0.091363	-0.038678	-0.009219	0.085310	0.030212
-0.156653	0.040311	0.016930	-0.025050	0.142583
-0.163008	0.055570	0.023212	-0.137038	-0.043257

-0.213214	0.007730	0.003559	0.153802	0.067321
0.130649	-0.003553	0.005490	-0.227677	-0.132793
0.003085	-0.279191	-0.150200	-0.074751	0.151789
-0.053087	0.111942	0.071889	0.142185	-0.087105
-0.262076	-0.054575	-0.036913	0.105194	-0.185673
-0.106933	-0.160137	-0.227703	-0.087210	-0.027619

-0.289967	-0.005510	-0.010457	-0.087577	0.091541
0.373375	0.014174	0.015608	0.161050	-0.248053
0.012192	0.305525	0.112627	0.289878	-0.166114
0.225370	0.320015	-0.078573	0.193438	-0.243933
-0.357474	0.041423	-0.111999	-0.213617	0.131339
0.414593	-0.457326	0.249102	0.338144	0.106575

-0.020890	0.000183	-0.000274	0.004042	0.022394
-0.042332	-0.000323	0.000243	-0.012565	0.017244
-0.000120	0.021228	-0.023631	-0.043927	-0.006830
-0.007497	0.034379	0.051715	-0.002944	-0.005907
0.000038	0.080812	0.045017	-0.039922	0.028705
-0.023357	-0.013549	-0.048462	0.053329	0.056896

-0.062137	-0.003451	0.000394	-0.011193	0.066292
-0.031813	-0.003794	0.000465	0.034795	0.051183
-0.003352	-0.030000	0.065442	-0.013704	0.009816
-0.002367	0.067608	-0.074298	-0.008730	-0.011535
0.024652	-0.034776	0.085343	0.057356	-0.074493
-0.017285	-0.035339	0.060652	0.016640	0.017745

-0.127922	0.000014	0.000168	0.020219	0.136525
-0.045240	0.000178	0.000249	-0.062855	0.105406
-0.000638	-0.012774	-0.115219	0.112845	0.004090
0.019289	0.037285	-0.031150	-0.018015	-0.006292
0.056832	0.163149	0.047354	0.024044	0.143603
0.059996	-0.019809	0.020203	-0.137005	-0.145186

-0.213127	-0.001093	-0.001293	-0.025147	0.227426
0.150711	0.004091	-0.000746	0.081285	0.175535
-0.001194	0.000000	0.152590	0.071754	-0.032043
0.012343	-0.107650	0.242355	-0.030060	0.018464
0.001912	-0.148884	-0.141006	-0.137467	-0.185723
0.038140	0.057343	-0.227675	-0.067120	-0.092940

-0.287862	0.000000	0.0001615	0.018494	0.309197
0.373333	-0.001013	-0.000096	-0.057512	0.238605

-0.001740	-0.001740	-0.108178	-0.278475	0.035080
-0.017049	-0.107087	-0.865353	-0.041927	0.092367
0.120338	0.140187	-0.401383	0.215212	0.131416
-0.142237	0.163813	0.242237	0.778143	0.360618

SOLUTION OF THE DISPERSION MODEQUATION USING ORDINARY B.C.

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	0.528624	0.187825	0.040081	0.010254	0.001767
0.2	0.731426	0.419465	0.191824	0.072025	0.024543
0.3	0.828303	0.585721	0.350340	0.179504	0.086911
0.4	0.883242	0.698711	0.488136	0.302727	0.182205
0.5	0.916835	0.775528	0.598834	0.421783	0.293073
0.6	0.934980	0.831490	0.685544	0.527739	0.404557
0.7	0.944273	0.871280	0.753062	0.617936	0.507556
0.8	0.952203	0.900698	0.805684	0.692960	0.597896
0.9	0.958210	0.922823	0.846815	0.754262	0.674554
1.0	0.973216	0.933685	0.879061	0.803692	0.738205

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	0.528578	0.187812	0.049077	0.010253	0.001767
0.2	0.731380	0.419429	0.191806	0.072018	0.024541
0.3	0.828748	0.585671	0.350309	0.179488	0.086904
0.4	0.883184	0.698654	0.488096	0.302704	0.182194
0.5	0.916776	0.775467	0.593789	0.421756	0.293061
0.6	0.936920	0.831428	0.685497	0.527710	0.404543
0.7	0.954212	0.871217	0.753215	0.617957	0.507550
0.8	0.965142	0.900635	0.805636	0.692933	0.597895
0.9	0.973148	0.922760	0.846767	0.754236	0.674557
1.0	0.979155	0.939623	0.879014	0.803367	0.738212

CONCENTRATIONS AT GRID POINTS

TIME	11	12	13	14	15
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	0.527637	0.187842	0.049086	0.010255	0.001767
0.2	0.731504	0.419535	0.191863	0.072041	0.024551
0.3	0.829916	0.585851	0.350437	0.179561	0.086952
0.4	0.883379	0.698823	0.488296	0.302843	0.182309
0.5	0.916890	0.775750	0.599052	0.421967	0.293264
0.6	0.939147	0.831743	0.685812	0.527990	0.404845
0.7	0.954640	0.871556	0.753372	0.618309	0.507940
0.8	0.965365	0.900993	0.806028	0.693127	0.598363
0.9	0.973437	0.922131	0.847185	0.754675	0.675193
1.0	0.979408	0.940005	0.879454	0.804342	0.738820

CONCENTRATIONS AT GRID POINTS					
TIME	15	17	18	19	20
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	0.523629	0.187856	0.049084	0.010054	0.001767
0.2	0.731477	0.413511	0.191850	0.072036	0.024549
0.3	0.823377	0.585308	0.350405	0.179543	0.086943
0.4	0.823333	0.693834	0.488245	0.302308	0.182288
0.5	0.915939	0.776678	0.538983	0.421512	0.293226
0.6	0.829091	0.831661	0.635727	0.527916	0.404789
0.7	0.954300	0.871466	0.753273	0.618217	0.507865
0.8	0.965324	0.900896	0.805917	0.693220	0.598276
0.9	0.973244	0.923029	0.847065	0.754554	0.674996
1.0	0.979343	0.933398	0.879325	0.804210	0.738699

CONCENTRATIONS AT GRID POINTS					
TIME	21	22	23	24	25
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	0.523575	0.187810	0.049077	0.010053	0.001767
0.2	0.731371	0.413420	0.191800	0.072016	0.024542
0.3	0.823732	0.585650	0.350292	0.179479	0.086909
0.4	0.833152	0.693621	0.488064	0.302683	0.182207
0.5	0.916740	0.776422	0.598741	0.421721	0.293081
0.6	0.933528	0.831372	0.685433	0.527661	0.404574
0.7	0.954178	0.871152	0.752937	0.617904	0.507582
0.8	0.965104	0.900553	0.805546	0.692856	0.597930
0.9	0.973118	0.922681	0.846566	0.754148	0.674594
1.0	0.979113	0.933539	0.878904	0.803768	0.738250

CONCENTRATIONS AT GRID POINTS					
TIME	26	27	28	29	30
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	0.523509	0.187827	0.049082	0.010054	0.001767
0.2	0.731442	0.413481	0.191833	0.072029	0.024544
0.3	0.823829	0.585754	0.350366	0.179519	0.086919
0.4	0.833274	0.693758	0.488179	0.302757	0.182225
0.5	0.916672	0.776585	0.598691	0.421629	0.293106
0.6	0.933019	0.831553	0.685611	0.527747	0.404605
0.7	0.954314	0.871346	0.753135	0.618062	0.507613
0.8	0.965248	0.900767	0.805750	0.693031	0.597959
0.9	0.973261	0.922892	0.846892	0.754334	0.674617
1.0	0.979258	0.933755	0.875128	0.803952	0.738267

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.528611	0.187829	0.049082	0.010054	0.001767
0.2	0.731448	0.414487	0.191837	0.072031	0.024547
0.3	0.823830	0.585768	0.350377	0.179528	0.086935
0.4	0.833290	0.695782	0.438202	0.302780	0.182271
0.5	0.816891	0.776618	0.598929	0.421872	0.293198
0.6	0.939042	0.831595	0.685665	0.527966	0.404751
0.7	0.954348	0.871397	0.753205	0.618160	0.507821
0.8	0.965273	0.908825	0.805846	0.693159	0.598228
0.9	0.973202	0.922958	0.846993	0.754491	0.674946
1.0	0.978291	0.939827	0.879253	0.804148	0.738651

WEIGHTED AVERAGE

TWO DIMENSIONAL HOMOGENEOUS CASE

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.528605	0.187826	0.049081	0.010054	0.001767
0.2	0.731435	0.415475	0.191830	0.072028	0.024545
0.3	0.823819	0.585745	0.350360	0.179517	0.086925
0.4	0.833265	0.698748	0.486172	0.302756	0.182242
0.5	0.816882	0.776574	0.598885	0.421831	0.293142
0.6	0.939010	0.831544	0.685606	0.527805	0.404662
0.7	0.954305	0.871338	0.753134	0.618078	0.507695
0.8	0.965235	0.908760	0.805762	0.693055	0.598065
0.9	0.973253	0.922887	0.846897	0.754367	0.674748
1.0	0.979250	0.939751	0.879147	0.804005	0.728419

ABSOLUTE DEVIATION

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	-0.000000
0.1	-0.000006	-0.000003	-0.000001	-0.000000	0.000000
0.2	-0.000013	-0.000012	-0.000007	-0.000013	-0.000002
0.3	-0.000023	-0.000023	-0.000017	-0.000011	-0.000010
0.4	-0.000025	-0.000034	-0.000030	-0.000024	-0.000029
0.5	-0.000029	-0.000044	-0.000044	-0.000041	-0.000056
0.6	-0.000032	-0.000051	-0.000059	-0.000061	-0.000089
0.7	-0.000035	-0.000059	-0.000071	-0.000082	-0.000126
0.8	-0.000038	-0.000065	-0.000084	-0.000104	-0.000163
0.9	-0.000039	-0.000071	-0.000096	-0.000124	-0.000198
1.0	-0.000041	-0.000076	-0.000106	-0.000143	-0.000232

PERCENT DEVIATION

TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	-0.001679	-0.001853	-0.001497	-0.003430	0.001074
0.2	-0.001811	-0.002023	-0.003671	-0.004286	-0.006855
0.3	-0.002362	-0.003940	-0.004888	-0.006139	-0.011939
0.4	-0.002876	-0.004829	-0.006230	-0.007991	-0.015811
0.5	-0.003129	-0.005616	-0.007421	-0.009805	-0.019102
0.6	-0.003436	-0.006135	-0.008551	-0.011631	-0.021993
0.7	-0.003718	-0.006727	-0.009445	-0.013297	-0.024854
0.8	-0.003894	-0.007201	-0.010379	-0.014951	-0.027187
0.9	-0.004048	-0.007707	-0.011282	-0.016375	-0.029346
1.0	-0.004188	-0.008084	-0.012026	-0.017826	-0.031391

APPENDIX D

ONE DIMENSIONAL NON-HOMOGENEOUS CASE

The partial differential equation describing the above problem is:

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial}{\partial z} (D_L(z) \frac{\partial c}{\partial z}) - \frac{\partial c}{\partial z}.$$

The boundary conditions are:

$$\begin{aligned} \text{(a)} \quad & \text{at } z = 0, \quad c = 1 \\ & \text{at } z = 1, \quad \frac{\partial c}{\partial z} = 0 \end{aligned}$$

$$\text{(b)} \quad \text{at } z = 0, \quad c_{in}(\theta) = \alpha c_{z \rightarrow 0^+} - \alpha (D_L(z) \frac{\partial c}{\partial z})_{z \rightarrow 0^+}$$

The following values of the parametes were used

$$\alpha = 0.3$$

$$D_L(z) = 0.5 (1.0 + z).$$

Semi Analytical Solution A ten point and a twenty point grid are used for solving the above problem. $0 \leq z \leq 1$. The grid spacing used is shown in the Figure III-f.

Interpolated Values The results of the ten point grid are derived from those of the twenty point grid using Legrangian Interpolation formula.

Deviations (Errors) The accuracy of the solution can be checked to some extent from the deviations between the interpolated value and the value given by the semi analytical solution.

ie Deviation = Interpolated Value - The value given by semi analytical solution.


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C      SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C      DIMENSIONAL NON-HOMOGENEOUS CASE
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
C      ASSUMED DATA
C      LINEAR RELATIONSHIP OF D VS Z   D=0.5(1.0+Z)
C      D= AXIAL DISPERSION COEFFICIENT.
C      Z= DIMENSIONLESS LENGTH.
C      ALPHA= 1.0/(U*L) AND IS ASSUMED AS 0.3
C      U= VELOCITY OF THE FLOWING FLUID.
C      L= REACTOR LENGTH.
C      BETA= GRID SPACING/2.0 =0.04762
C      DOUBLE PRECISION MATRIX(20,20),VECTOR(20,20),
1TOLERC,W(20,20),CEVR(20,20),TIME(20)
C      DOUBLE PRECISION X(20),VAR(20),CI(20),C1(20)
C      DOUBLE PRECISION D(20,20),VICTOR(20,20)
C      READ( 5,1)  N,NT
C      READ(5,5)  ((MATRIX(I,J),J=1,N),I=1,N)
C      READ( 5,2 )  (X(J),J=1,N)
C      READ( 5,2 )  (CI(J),J=1,N)
C      READ( 5,2 )  (C1(J),J=1,N)
C      READ(5,3)  (TIME(J), J=1,NT)
C      READ(5,6)  ((D(I,J),J=1,N),I=1,N)
C      READ(5,4) DX
C      NORM=2
C      TOLERC=0.000
C      WRITE(6,222)
C      LINES=9
C      CALL LINECT(LINES,4,2)
C      WRITE(6,252)
C      WRITE(6,201)  N,NT
C      WRITE(6,223)
C      LINES=9
C      CALL LINECT(LINES,4,2)
C      WRITE(6,253)  DX
C      WRITE(6,220)
C      LINES =9
C      CALL LINECT(LINES,4,2)
C      WRITE(6,224)
C      WRITE(6,223)
C      WRITE(6,231)
C      CALL LINECT(LINES,1,2)
C      WRITE(6,232)  (X(J),J=1,N)

```



```

CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,233)
CALL LINECT(LINES,2,2)
WRITE(6,234) (C1(J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,235)
CALL LINECT(LINES,2,2)
DO 30 J=1,N
30 C1(J)=C1(J)/(DX**2)
WRITE(6,234) (C1(J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,240)
DO 35 J=1,N
DO 35 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(DX**2)
35 CONTINUE
DO 31 J=1,N
CALL LINECT(LINES,1,2)
31 WRITE(6,241) (MATRIX(J,K),K=1,N)
CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NORM)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,242)
CALL LINECT(LINES,2,2)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,243)
DO 32 K=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
32 WRITE(6,223)
CALL CHECK(VECTOR,MATRIX,N,W)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,1,2)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (W(J,K),K=1,N)
33 WRITE(6,223)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,4,2)
WRITE(6,255)

```



```

DO 37 J=1,N
CALL LINECT(LINES,1,2)
WRITE(6,241) (D(J,K),K=1,N)
37 WRITE(6,223)
C CALCULATE THE TRANSPOSE OF THE MATRIX OF
C THE EIGENVECTORS
DO 40 I=1,N
DO 40 J=1,N
VICTOR(I,J)=VECTOR(J,I)
40 CONTINUE
WRITE(6,220)
LINES=9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,258)
DO 42 K=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (VICTOR(K,J),J=1,N)
42 WRITE(6,223)
C A=(D(-1)*A(*)*D)
C A(*)=THE ORIGINAL COEFFICIENT MATRIX
C D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C COEFFICIENT MATRIX A(*)
C Q=THE MATRIX OF EIGENVECTORS OF A
C CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C COEFFICIENT MATRIX
DO 38 I=1,N
DO 38 J=1,N
VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
WRITE(6,220)
LINES=9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,256)
CALL LINECT(LINES,2,2)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,257)
DO 39 K=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
C (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
C QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
C D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
C CALCULATE THE PRODUCT (QT*D(-1))

```



```

DO 41 I=1,N
DO 41 J=1,N
VICTOR(I,J)=VICTOR(I,J)/D(J,J)
41 CONTINUE
CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
1CEVR,VICTOR)
WRITE(6,220)
WRITE(6,225)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,248)
DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)
WRITE(6,249)
DO 36 J=1,NT
36 WRITE(6,251) TIME(J), (CEVR(J,K),K=6,10 )

```

C FORMAT STATEMENTS

```

1  FORMAT(1X,2I4)
2  FORMAT(10F8.5)
3  FORMAT(11F7.3)
4  FORMAT(1X,F16.8)
5  FORMAT(10F8.6)
6  FORMAT(5F16.8)
201 FORMAT(1H,10X,3H N=, 13,10X,3HNT=, 13)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
111HDIMENSIONAL/25X,22HNON HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
18HEQUATION/20X,21HUSING DANCKWERTS B.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,19H COEFFICIENT MATRIX)
241 FORMAT(1H,10X,10F5.1)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,

```



```
18X,2H 9, 8X, 2H10)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
252 FORMAT(1H,5X,12HGRID POINTS ,2X,15HNUMBER OF TIMES)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
255 FORMAT(1H,10X,9HMATRIX(D))
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
127HORIGINAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
127HORIGINAL COEFFICIENT MATRIX)
258 FORMAT(1H,20X,26HTRANSPOSE OF THE MATRIX OF,
112HEIGENVECTORS)
STOP
END
```


45 10 POINTS

INITIAL CONDITION VECTOR

BOUNDARY CONDITION VECTOR

COEFFICIENT MATRIX

[illegible]

EIGENVALUES

2.115763	137.125419	6.483325	37.969677	64.555529
90.063057	14.243724	51.500352	76.324725	25.165926

EIGENVECTORS

0.033102	0.001012	-0.244873	-0.343090	-0.327534
-0.029400	0.373393	-0.452995	0.146543	0.461548

-0.184284	0.007077	0.401077	-0.347428	-0.511271
-0.087184	-0.449938	-0.381131	0.527687	-0.281072

0.256951	0.022066	-0.441923	0.455790	-0.347817
-0.195367	0.223433	0.182287	0.485079	-0.221696

-0.314537	0.061534	0.373101	-0.053293	0.112371
-0.355295	0.117740	0.428518	0.475125	0.439420

0.355789	0.143143	-0.223858	-0.405882	0.417216
-0.502245	-0.270599	-0.060869	0.190953	-0.185048

-0.330222	0.231687	0.035764	0.228381	0.151268
-0.508255	0.408432	-0.407239	-0.227246	-0.233190

0.337484	0.459426	0.147251	0.253807	-0.313892
-0.265609	-0.037109	0.064379	-0.393765	0.411195

-0.378411	0.504810	-0.292087	-0.374930	-0.258481
0.146531	-0.038377	0.375983	-0.092256	-0.222079

0.354672	0.536726	0.372285	0.013823	0.241552
0.400046	0.281062	-0.147220	0.314061	-0.139134

-0.318071	0.337722	-0.383077	0.445585	0.260740
0.233238	-0.340019	-0.309874	0.243358	0.373283

CHECK OF SIMILARITY TRANSFORMATION

36.223410	18.157457	0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

18.157457	39.473664	19.789942	0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000

0.000000	19.789942	42.523577	21.415216	-0.000000
0.000000	-0.000000	0.000000	0.000000	0.000000

0.000000	0.000000	21.415216	45.673446	23.641334
0.000000	-0.000000	0.000000	0.000000	-0.000000

0.000000	-0.000000	-0.000000	23.641334	46.823384
24.645413	0.000000	0.000000	-0.000000	-0.000000

0.000000	-0.000000	0.000000	0.000000	24.645413
51.973323	26.293585	0.000000	-0.000000	-0.000000

0.000000	-0.000000	-0.000000	-0.000000	0.000000
26.293585	55.123261	27.859073	0.000000	0.000000

-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	27.859073	58.273200	29.479584	0.000000

-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	29.479584	51.419831	31.056197

-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	31.056197	35.745644

MATRIX(D)

-1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 -1.7 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 -2.3 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 3.4 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 -4.2 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 5.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -6.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 7.1

TRANSPOSE OF THE MATRIX OF EIGENVECTORS

0.094108	-0.188289	0.255951	-0.314537	0.355789
-0.382222	0.387484	-0.373411	0.354672	-0.318071

0.001812	0.507077	0.022506	0.261534	0.143140
0.281087	0.455425	0.584810	0.538726	0.237122

-0.244873	0.401077	-0.441923	0.373101	-0.223858
0.035754	0.147951	-0.292067	0.373285	-0.383077

-0.493090	-0.047428	0.455799	-0.253093	-0.405880
0.228381	0.258607	-0.374900	0.013623	0.345583

-0.327534	-0.511071	-0.349817	0.112371	0.417216
0.161268	-0.313022	-0.258481	0.241552	0.269749

-0.029400	-0.087184	-0.195367	-0.355395	-0.502245
-0.508255	-0.265809	0.146531	0.409040	0.238238

0.373393	-0.400938	0.226489	0.117740	-0.370599
0.403402	-0.237109	-0.038377	0.281262	-0.380919

-0.452995	-0.301131	0.162087	0.428518	-0.050869
-0.407239	0.064379	0.575983	-0.147220	-0.309874

0.145543	0.327080	0.485679	0.475125	0.190953
-0.227246	-0.308765	-0.092256	0.314061	0.243358

0.461548	-0.231072	-0.221696	0.439420	-0.185048
-0.233190	0.411195	-0.222079	-0.130184	0.373283

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

2.112760	127.125319	6.483325	37.269877	64.555529
30.063257	14.342724	51.502352	76.824725	25.165926

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.098108	-0.081812	0.244373	0.493092	0.327534
0.023420	-0.373393	0.452945	-0.146543	-0.461548

-0.245174	0.009412	0.533433	-0.263079	-0.679724
-0.115955	-0.598417	-0.506924	0.435814	-0.373826

-0.444238	-0.239017	0.764085	-0.768076	0.604834
0.330518	-0.391620	-0.314828	-0.339739	0.383312

-0.693555	0.136723	0.822688	-0.117069	0.247777
-0.733647	0.259618	0.944882	1.047650	0.968921

-0.933750	-0.295782	0.613968	1.122259	-1.153601
1.388709	1.024726	0.168302	-0.527935	0.511657

-1.239597	0.360755	0.122242	0.780627	0.551216
-1.737217	1.395917	-1.391942	-0.776725	-0.797043

-1.615805	-1.397122	-0.615957	-1.279225	1.308928
1.107589	0.988744	-0.263459	1.642022	-1.714583

-1.903027	2.241225	-1.468853	-1.385374	-1.299900
0.736903	-0.192996	1.890317	-0.463956	-1.116634

-2.138674	-3.248515	-2.250906	-0.202146	-1.456557
-2.465545	-1.696011	0.687738	-1.393791	0.830270

-2.263803	1.645170	-2.732488	2.465042	1.924117
1.699349	-2.781230	-2.210331	1.735871	2.662631

SOLUTION OF THE DISPERSION MODEL EQUATION
USING ORDINARY O.C.
SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS					
TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.735698	0.460559	0.248723	0.118527	0.050751
0.2	0.862388	0.687810	0.507699	0.348427	0.223532
0.3	0.913159	0.795308	0.659653	0.521595	0.393846
0.4	0.947137	0.855966	0.752393	0.641761	0.527633
0.5	0.966532	0.894047	0.815234	0.725082	0.629212
0.6	0.977354	0.919724	0.858308	0.786140	0.706879
0.7	0.979924	0.937956	0.889612	0.831860	0.767118
0.8	0.982449	0.951413	0.913109	0.866914	0.814444
0.9	0.984612	0.961633	0.931169	0.894261	0.851986
1.0	0.987820	0.969555	0.945286	0.915859	0.881968

CONCENTRATIONS AT GRID POINTS					
TIME	6	7	8	9	10
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.019846	0.007185	0.002429	0.000786	0.000261
0.2	0.134939	0.077163	0.042147	0.022857	0.014034
0.3	0.286050	0.193765	0.134991	0.093113	0.071142
0.4	0.421370	0.323199	0.252303	0.198584	0.168586
0.5	0.534381	0.446399	0.370885	0.315694	0.283729
0.6	0.625910	0.548228	0.479476	0.428642	0.398456
0.7	0.699773	0.633641	0.574010	0.530062	0.500203
0.8	0.759197	0.704233	0.654007	0.617383	0.594363
0.9	0.807210	0.762232	0.720577	0.690837	0.671507
1.0	0.845991	0.809576	0.775403	0.751746	0.735713

CONCENTRATION PROFILES-ONE-DIMENSIONAL NON HOMOGENEOUS MEDIUM

GRID POINTS

0.295240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

8.5187	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

COEFFICIENT MATRIX

[illegible]

EIGENVALUES

1.738732	107.125281	4.809068	35.109130	76.613811
11.628331	49.424361	90.058756	63.540162	22.051930

EIGENVECTORS

0.265306	0.001492	-0.449014	-0.390716	-0.102273
-0.469555	0.316726	-0.022512	-0.218368	0.442594

-0.298536	0.006981	0.429327	-0.278418	-0.306655
0.272620	0.475399	-0.084170	-0.497527	-0.002888

0.324323	0.022532	-0.337889	0.418498	-0.483240
0.048614	-0.049158	-0.194926	-0.407221	-0.403574

-0.341798	0.061520	0.198331	0.112384	-0.485887
-0.322053	-0.455142	-0.354897	0.060106	0.388459

0.350300	0.143133	-0.037702	-0.440491	-0.203323
0.430672	-0.028404	-0.502481	0.425089	-0.023149

-0.349689	0.281084	-0.118090	0.140047	0.224993
-0.348882	0.424826	-0.508926	0.197644	-0.338030

0.339749	0.455426	0.247163	0.323056	0.401426
0.131649	-0.014560	-0.266180	-0.311498	0.406367

-0.321000	0.584813	-0.334929	-0.364262	0.097311
0.123739	-0.397975	0.146537	-0.280649	-0.163360

0.294524	0.538730	0.373849	-0.019072	-0.318817
-0.320201	0.133219	0.409545	0.244232	-0.183309

-0.261285	0.237724	-0.363543	0.361929	-0.248349
0.395912	0.326317	0.238570	0.283077	0.387436

CHECK OF SIMILARITY TRANSFORMATION

22.170398	18.157457	-0.000000	0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000

18.157457	39.373569	19.789092	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000

-0.000000	19.789092	42.523507	21.415216	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000

0.000000	-0.000000	21.415216	45.673446	23.041339
0.000000	-0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	0.000000	23.041339	48.823384
24.645413	-0.000000	-0.000000	-0.000000	-0.000000

0.000000	-0.000000	-0.000000	0.000000	24.645413
51.973323	26.293585	0.000000	-0.000000	-0.000000

0.000000	-0.000000	-0.000000	-0.000000	-0.000000
26.293585	55.123261	27.859073	0.000000	-0.000000

-0.000000	0.000000	0.000000	0.000000	-0.000000
0.000000	27.859073	58.273200	29.479684	0.000000

-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	29.479684	61.419831	31.056197

0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	31.056197	36.745644

MATRIX(D)

-1.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 1.3 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 -1.7 0.0 0.0 0.0 0.0 0.0 0.0 0.0

0.0 3.0 0.0 2.2 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.0 0.0 -2.8 0.0 0.0 0.0 0.0 0.0

0.0	0.0	0.0	0.0	0.0	3.4	0.0	0.0	0.0	0.0
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

0.0 0.0 0.0 0.0 0.0 0.0 -4.2 0.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 5.0 0.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -6.0 0.0

0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 7.1

TRANSPOSE OF THE MATRIX OF EIGENVECTORS

0.265306	-0.298536	0.324323	-0.341798	0.350300
-0.349689	0.339749	-0.321000	0.294524	-0.261285

0.001492	0.006981	0.022532	0.061520	0.143133
0.281784	0.455426	0.584813	0.538730	0.237724

-0.449014	0.429327	-0.337889	0.198331	-0.037702
-0.118090	0.247163	-0.334929	0.373849	-0.363543

-0.390716	-0.278418	0.418498	0.112384	-0.440491
0.140047	0.323756	-0.364262	-0.019072	0.361929

-0.102273	-0.306655	-0.483240	-0.485887	-0.203323
0.224993	0.401426	0.097311	-0.318817	-0.248349

-0.469555	0.272620	0.048614	-0.322053	0.430672
-0.348882	0.131649	0.123739	-0.320201	0.395912

0.316726	0.475399	-0.049158	-0.455142	-0.028404
0.424826	-0.014560	-0.397975	0.133219	0.326317

-0.022512	-0.084170	-0.194926	-0.354897	-0.502481
-0.508926	-0.266180	0.146537	0.409545	0.238570

-0.218368	-0.497527	-0.407221	0.060106	0.425089
0.197644	-0.311498	-0.280649	0.244232	0.283077

0.442594	-0.002888	-0.403574	0.388459	-0.023149
-0.338030	0.406367	-0.163360	-0.183309	0.387436

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

1.738732	107.125231	4.809068	35.109130	76.613811
11.628331	49.424361	90.058756	63.540162	22.051930

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.265306	-0.001492	0.449014	0.390716	0.102273
0.469555	-0.316726	0.022512	0.218368	-0.442594

-0.397053	0.009285	0.571005	-0.370296	-0.407850
0.362584	0.632281	-0.111946	-0.661711	-0.003841

-0.560754	-0.038958	0.584210	-0.723583	0.835522
-0.084054	0.084995	0.337027	0.704085	0.697779

-0.753666	0.135651	0.437319	0.247808	-1.071381
-0.710127	-1.003587	-0.782548	0.132535	0.856552

-0.968578	-0.395764	0.104246	1.217957	0.562189
-1.190808	0.078536	1.389360	-1.175372	0.064006

-1.195238	0.960747	-0.403632	0.478680	0.769027
-1.192477	1.452054	-1.739509	0.675547	-1.155388

-1.416754	-1.899126	-1.030672	-1.347143	-1.673947
-0.548978	0.060717	1.109969	1.298945	-1.694550

-1.614310	2.941024	-1.684359	-1.831876	0.489376
0.622285	-2.001416	0.736933	-1.411382	-0.821539

-1.775979	-3.248541	-2.254310	0.115004	1.922465
1.930815	-0.803310	-2.469558	-1.472716	1.105353

-1.863748	1.695682	-2.593155	2.581640	-1.771476
2.824038	2.327616	1.701721	2.019186	2.763583

SOLUTION OF THE DISPERSION MODEL EQUATION
 USING DANCKWERTS B.C.
 SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS					
TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.430437	0.249537	0.127341	0.058121	0.024076
0.2	0.604319	0.451520	0.314881	0.205828	0.126674
0.3	0.707003	0.584317	0.461551	0.349038	0.253152
0.4	0.775370	0.676795	0.571764	0.467913	0.371284
0.5	0.823811	0.744029	0.655500	0.563679	0.473448
0.6	0.859530	0.794473	0.720226	0.640712	0.559699
0.7	0.886636	0.833253	0.771095	0.703052	0.631994
0.8	0.907670	0.863650	0.811655	0.753878	0.692497
0.9	0.924285	0.887854	0.844384	0.795600	0.743144
1.0	0.937596	0.907368	0.871050	0.830042	0.785572

CONCENTRATIONS AT GRID POINTS					
TIME	6	7	8	9	10
0.0	-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.1	0.009171	0.003251	0.001080	0.000344	0.000121
0.2	0.073799	0.040934	0.021766	0.011519	0.006928
0.3	0.176695	0.119232	0.078560	0.052683	0.039394
0.4	0.286531	0.216108	0.161141	0.123341	0.102668
0.5	0.389645	0.315797	0.254903	0.211463	0.186821
0.6	0.481683	0.410360	0.349545	0.305454	0.279780
0.7	0.561934	0.496312	0.439112	0.397463	0.372655
0.8	0.631035	0.572492	0.520656	0.483053	0.460147
0.9	0.690092	0.638934	0.593085	0.560163	0.539612
1.0	0.740318	0.696262	0.656373	0.628190	0.610095

SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
 DIMENSIONAL NON-HOMOGENEOUS CASE

INPUT DATA

N= THE NUMBER OF GRID POINTS.

NT = THE TOTAL NO. OF TIMES.

MATRIX=THE COEFFICIENT MATRIX

X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.

CI= THE INITIAL CONDITION VECTOR.

C1= THE BOUNDARY CONDITION VECTOR.

TIME= THE DIMENSIONLESS TIMES.

DX= THE GRID SPACING.

ASSUMED DATA

LINEAR RELATIONSHIP OF D VS Z $D=0.5(1.0+Z)$.

D= THE AXIAL DISPERSION COEFFICIENT.

Z= THE DIMENSIONLESS LENGTH.

ALPHA= $1.0/(U*L)$ AND IS ASSUMED AS 0.3

U= THE VELOCITY OF THE FLOWING FLUID.

L= THE REACTOR LENGTH.

BETA=GRID SPACING/2.0

DOUBLE PRECISION MATRIX(40,40),VECTOR(40,40),

1 TOLERC,W(40,40),CEVR(40,40),TIME(40)

DOUBLE PRECISION X(40),VAR(40),CI(40),C1(40)

DOUBLE PRECISION D(40,40),VICTOR(40,40)

READ THE DATA

READ(5,1) N,NT

READ(5,5) ((MATRIX(I,J),J=1,N),I=1,N)

READ(5,2) (X(J),J=1,N)

READ(5,2) (CI(J),J=1,N)

READ(5,2) (C1(J),J=1,N)

READ(5,3) (TIME(J), J=1,NT)

READ(5,6) ((D(I,J),J=1,N),I=1,N)

READ(5,4) DX

NORM=2

TOLERC=0.000

WRITE(6,223)

LINES=9

CALL LINECT(LINES,4,2)

WRITE(6,253) DX

WRITE(6,220)

LINES =9

CALL LINECT(LINES,4,2)

WRITE(6,224)

WRITE(6,223)

WRITE(6,231)

CALL LINECT(LINES,1,2)

WRITE(6,232) (X(J),J=1,N)

CALL LINECT(LINES,4,2)

WRITE(6,223)

WRITE(6,233)

CALL LINECT(LINES,2,2)


```

WRITE(6,234) (C1(J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,235)
CALL LINECT(LINES,2,2)
DO 30 J=1,N
30 C1(J)=C1(J)/(DX**2)
WRITE(6,234) (C1(J),J=1,N)
DO 36 J=1,N
DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(DX**2)
36 CONTINUE
WRITE(6,220)
WRITE(6,240)
CALL LINECT(LINES,4,2)
DO 31 J=1,N
WRITE(6,241)(MATRIX(J,K),K=1,N)
31 CONTINUE
CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NORM)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,6,2)
WRITE(6,242)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,243)
DO 32 K=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
32 WRITE(6,223)
CALL CHECK(VECTOR,MATRIX,N,W)
CALL LINECT(LINES,1,2)
WRITE(6,223)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232) (W(J,K),K=1,N)
33 WRITE(6,223)
WRITE(6,220)
WRITE(6,255)
DO 37 J=1,N
WRITE(6,241) (D(J,K),K=1,N)
37 CONTINUE
CALCULATE THE TRANSPOSE OF THE MATRIX OF
THE EIGENVECTORS
DO 40 I=1,N
DO 40 J=1,N
VECTOR(I,J)=VECTOR(J,I)
40 CONTINUE

```



```

C      A=(D(-1)*A(*)*D)
C      A(*)=THE ORIGINAL COEFFICIENT MATRIX
C      D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C      OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C      A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C      COEFFICIENT MATRIX A(*)
C      Q=THE MATRIX OF EIGENVECTORS OF A
C      CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C      COEFFICIENT MATRIX
DO 38 I=1,N
DO 38 J=1,N
VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
WRITE(6,220)
LINES=9
CALL LINECT(LINES,6,2)
WRITE(6,256)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,257)
DO 39 K=1,N
CALL LINECT(LINES,7,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
(D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
CALCULATE THE PRODUCT (QT*D(-1))
DO 41 I=1,N
DO 41 J=1,N
VICTOR(I,J)=VICTOR(I,J)/D(J,J)
41 CONTINUE
CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
1CEVR,VICTOR)
WRITE(6,220)
WRITE(6,225)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,248)
DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)
WRITE(6,249)
DO 35 J=1,NT
35 WRITE(6,251) TIME(J), (CEVR(J,K),K=6,10 )
WRITE(6,220)
WRITE(6,246)

```



```

WRITE(6,259)
DO 45 J=1,NT
45 WRITE(6,251) TIME(J), (CEVR(J,K),K=11,15)
WRITE(6,223)
WRITE(6,246)
WRITE(6,260)
DO 46 J=1,NT
46 WRITE(6,251) TIME(J), (CEVR(J,K),K=16,20)

```

C FORMAT STATEMENTS

```

1  FORMAT(1X,2I4)
2  FORMAT(10F8.5)
3  FORMAT(11F7.3)
4  FORMAT(1X,F16.8)
5  FORMAT(10F8.6)
6  FORMAT(10F8.4)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
      111HDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,19HUSING ORDINARY B.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,19H COEFFICIENT MATRIX)
241 FORMAT(1H,10X,10F6.1)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
      12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
      18X,2H 9, 8X, 2H10)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
255 FORMAT(1H,10X,9HMATRIX(D))
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
      127HORIGIONAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
      127HORIGIONAL COEFFICIENT MATRIX)
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,
      18X,2H14,8X,2H15)
260 FORMAT(1H,15X,5H TIME,9X,2H16,8X,2H17,8X,2H18,
      18X,2H19,8X,2H20)

```


D-26

STOP
END

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.043780	0.027060	0.145340	0.195120	0.243900
0.292680	0.341460	0.390240	0.439020	0.487800
0.536580	0.585360	0.634140	0.682920	0.731700
0.780480	0.829260	0.878040	0.926820	0.975600

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

74.9228	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

COEFFICIENT MATRIX

EIGENVALUES

2.162730	443.784330	161.884075	399.287672	8.676245
43.527734	264.215301	266.512225	135.734533	15.137789
335.826195	365.043443	109.128375	17.513651	309.988731
62.745961	182.957406	240.604543	215.449007	34.844646

EIGENVECTORS

0.036809	0.000000	-0.355759	0.000013	-0.094031
-0.254965	-0.152857	-0.067628	-0.358920	-0.151769
-0.003098	-0.002869	0.343326	0.205274	-0.019534
0.294990	-0.237207	0.238538	-0.299674	-0.327942

-0.071606	0.000001	-0.157812	0.000053	0.176574
0.337055	-0.381296	-0.156716	-0.015277	0.265788
-0.009313	-0.001056	-0.120505	-0.322324	-0.049278
-0.306334	-0.286294	0.286666	-0.275271	0.231766

0.124226	0.000004	0.286921	0.000186	-0.242503
-0.214124	-0.394970	-0.265714	0.343687	-0.323111
-0.023359	-0.002493	-0.282953	0.314042	-0.106155
0.049714	0.115420	0.337066	-0.124634	0.135194

-0.134477	0.000014	0.210251	0.000593	0.283367
-0.026792	-0.357651	-0.266836	-0.030137	0.317587
-0.052232	-0.002037	0.252418	-0.194217	-0.136384
0.238483	0.366238	0.072934	0.236423	-0.332306

0.162173	-0.000051	-0.242979	0.001772	-0.312453
0.243089	-0.152773	-0.399316	-0.323497	-0.255084
-0.104539	-0.010756	0.123772	0.012737	-0.290824
-0.322126	0.060159	-0.237240	0.320533	0.157406

-0.187158	0.000171	-0.226132	0.004044	0.214651
-0.321638	0.186417	-0.100656	0.117013	0.150702
-0.185839	-0.000152	-0.323019	0.105845	-0.362753
0.152986	-0.000130	-0.322793	0.000084	0.176342

..CONTD

0.273263	0.000530	0.235840	0.012190	-0.235276
0.232499	0.314821	-0.066559	0.271326	-0.024957
-0.239310	-0.082007	0.082396	-0.264955	-0.403145
0.124085	-0.156115	-0.074004	-0.362213	-0.313781

-0.228370	0.001534	0.197946	0.028154	0.259810
-0.031497	0.217629	0.193368	-0.221853	-0.100288
-0.385117	-0.162135	0.253497	0.312251	-0.295477
-0.301710	0.258175	0.247295	-0.173316	0.144357

0.244355	0.004123	-0.253470	0.059443	-0.208622
-0.177433	-0.086769	0.313362	-0.161049	0.205398
-0.418889	-0.251194	-0.268818	-0.245903	-0.060356
0.263386	0.190520	0.253831	0.213036	0.163254

-0.257254	0.010265	-0.135166	0.114072	0.145665
0.297353	-0.237551	0.167562	0.295876	-0.275593
-0.333442	-0.366536	-0.032929	0.111174	0.200857
-0.049328	-0.233323	-0.075069	0.245539	-0.303331

0.264934	0.023659	0.286935	0.197350	-0.078189
-0.280358	-0.148996	-0.128176	-0.208255	0.302985
-0.116451	-0.433774	0.287200	0.050093	0.317847
-0.189825	-0.187695	-0.287547	-0.133553	0.174231

-0.273424	0.050275	0.033494	0.304092	0.007388
0.142361	0.171451	-0.283800	-0.281573	-0.285962
0.153803	-0.406453	-0.216475	-0.192745	0.183120
0.301751	0.235594	-0.065064	-0.268493	0.099163

0.276760	0.008043	-0.292642	0.409404	0.061637
0.051233	0.253374	-0.119318	0.168664	0.022614
0.320225	-0.241269	-0.033838	0.280543	-0.108370
-0.225744	0.158456	0.252494	0.088058	-0.286744

-0.277025	0.174335	0.036806	0.465462	-0.125270
-0.219242	-0.025120	0.183053	0.144334	-0.143822
0.250044	0.023657	0.288175	-0.204339	-0.285969
0.017095	-0.254264	0.147065	0.268201	0.237767

..CONTD

0.274258	0.280058	0.243453	0.415385	0.180440
0.293743	-0.259226	0.242898	-0.267352	0.041535
-0.022190	0.263272	-0.195718	0.234914	-0.155857
0.154143	-0.088897	-0.295181	-0.077319	-0.004131
-0.263654	0.400432	-0.209249	0.229605	-0.224746
-0.253758	-0.032636	-0.027650	0.076862	0.063223
-0.266703	0.333972	-0.085198	-0.120604	0.143338
-0.291459	0.272452	-0.184637	-0.258862	-0.226110
0.260347	0.500059	-0.121324	-0.049806	0.250501
0.119522	0.222340	-0.251406	0.218833	-0.157209
-0.240513	-0.153846	0.273127	-0.018852	0.263553
0.227051	-0.008594	0.174265	0.095833	0.282663
-0.249491	0.521193	0.275153	-0.295083	-0.274738
0.054902	0.144226	-0.093796	-0.254542	0.229504
0.042242	-0.147802	-0.206407	0.150300	0.035302
-0.043661	-0.265785	0.194664	0.239499	-0.133917
0.235276	0.411513	-0.054274	-0.353663	0.270220
-0.225233	-0.183716	0.205868	0.003564	-0.272582
0.269324	-0.008161	-0.050434	-0.244875	-0.235117
-0.157814	0.090212	-0.163517	-0.136104	-0.105079
-0.220919	0.162450	-0.232333	-0.162940	-0.270382
0.282361	-0.172221	-0.184640	0.244990	0.282863
0.162955	-0.102951	0.256259	0.283853	-0.163055
0.274104	0.218321	-0.188586	-0.202950	0.266066

CHECK OF SIMILARITY TRANSFORMATION

132.225913	66.858718	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
66.858915	130.274804	59.966828	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

..CONTD

-0.000000	67.948489	144.522675	73.078740	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	73.078740	150.675259	76.180248
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

-0.000000	-0.000000	-0.000000	76.180248	156.823640
79.281755	-0.000000	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000

-0.000000	-0.000000	-0.000000	-0.000000	79.281755
162.975221	82.383262	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	-0.000000	-0.000000
82.383262	169.124504	85.476364	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	85.476364	175.272485	38.573669	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

0.000000	0.000000	0.000000	-0.000000	0.000000
0.000000	-0.000000	38.573669	181.425554	91.666771
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	91.666771	187.573950
94.764078	-0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000

..CONTD

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	4.764075
193.725533	-7.857174	-0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
97.857174	199.814314	190.945277	-0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	100.945277	206.023295	104.039180	-0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000

0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	104.039180	212.175879	107.123079
-0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	107.123079	218.324260
110.212776	-0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	110.212776
224.475843	115.395378	-0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000
0.000000	-0.000000	0.000000	0.000000	-0.000000
113.305878	230.825224	115.395378	0.000000	0.000000

-0.000000	0.000000	0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	115.395378	230.825224	114.477475	-0.000000

..CONTD

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	119.479475	242.928189	122.563374

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	122.568574	133.251344

MATRIX(0)

EIGENVALUES OF THE ORIGINAL COEFFICIENT MATRIX

2.162732	442.744384	161.384275	342.287572	6.675245
43.527734	264.718491	226.512225	135.034503	15.137789
335.826198	345.049443	129.123875	27.613831	309.988731
62.795961	180.951476	243.603543	215.449090	64.844848

EIGENVECTORS OF THE ORIGINAL COEFFICIENT MATRIX

-0.036809	-0.000000	0.355759	-0.000013	0.094031
0.254065	0.157852	0.067508	0.358527	0.151767
0.003058	0.000000	-0.348326	-0.205804	0.018534
-0.294992	0.337227	-0.238538	0.299874	0.327042

-0.093421	0.000001	-0.183851	0.000062	0.205709
0.392269	-0.351202	-0.181759	-0.017565	0.302643
-0.010850	-0.001173	-0.140389	-0.375507	-0.057409
-0.355379	-0.333290	0.451469	-0.434860	0.270007

-0.145497	-0.000005	-0.385739	-0.000251	0.326894
0.283629	0.522420	0.358182	-0.463290	0.435554
0.031488	0.004821	0.381421	-0.423329	0.130053
-0.066071	-0.155386	-0.454365	0.168007	-0.182242

-0.208480	0.000022	0.339920	0.000926	0.447055
-0.041536	-0.554321	-0.563749	-0.046795	0.492355
-0.080970	-0.012467	0.391324	-0.301095	-0.288951
0.369720	0.533439	0.113100	0.366526	-0.516174

-0.287511	-0.000001	0.430752	-0.003141	0.553915
-0.430049	0.270235	0.707008	0.570495	0.452212
0.185327	0.035723	-0.237152	-0.022581	0.515573
0.571064	-0.110195	0.420543	-0.558330	-0.270160

-0.377442	0.000044	-0.455161	0.000704	0.634557
-0.648647	0.275119	-0.605333	0.237795	0.303920
-0.374762	-0.080061	-0.651433	0.354459	-0.771898
0.308325	-0.015970	-0.646943	0.019933	0.355630

..CONTD

-0.477765	-0.001011	-0.547706	-0.227937	0.275428
-0.530612	-0.718767	0.151061	-0.819454	0.058979
0.660524	0.303396	-0.183117	0.650583	0.920421
-0.283279	0.350634	0.168960	0.689495	0.727817
-0.587641	0.403446	0.509553	0.272447	0.683542
-0.081047	0.567004	0.510442	-0.570564	-0.258062
-0.990983	-0.417237	0.652248	0.803484	-0.761321
-0.775359	0.664436	0.636339	-0.445976	0.371461
-0.725800	-0.211392	0.745487	-0.171673	0.602522
0.512444	0.247707	-0.905020	0.465127	-0.593211
1.209794	-0.754356	0.776373	0.710206	0.174315
-0.760685	-0.556250	-0.733090	-0.615270	-0.462830
-0.830673	0.233145	-0.429679	0.368340	0.473581
0.960154	-0.024535	0.541059	0.255384	-0.890229
-1.076635	-1.183544	-0.106328	0.358980	0.048566
-0.159282	-0.755116	-0.242397	0.796075	-0.995602
-0.960189	-0.089105	-1.032135	-0.709884	0.231183
1.008477	0.535356	0.461063	0.029695	-1.030868
0.418884	1.560322	-1.033412	-0.130191	-1.143327
0.682810	0.675158	1.034335	0.480404	-0.644710
-1.091919	0.220774	0.153725	1.214393	0.029505
0.568520	0.684688	-1.133353	-1.124461	-1.141990
0.614214	-1.615132	-0.864492	-0.769727	0.731289
1.215041	0.047043	-0.259852	-1.071827	0.346007
-1.223112	-0.433893	1.293304	-1.809321	-0.272596
-0.225861	-1.114764	0.527313	-0.834667	-1.014754
-1.414316	1.065160	0.370760	-1.239333	0.478932
0.097652	-0.601441	-1.115871	-0.389165	1.267238
-1.350730	0.450490	0.423283	2.262687	-0.610840
-1.064160	-0.120491	0.892504	0.703602	-0.701305
1.219264	0.115357	1.405201	-1.435258	-1.324444
0.087745	-1.237041	0.717117	1.303730	1.159401

..CNT0

-1.471664	-1.532536	-1.336101	-2.228499	-0.968044
-1.575933	1.398366	-1.303124	1.541813	-0.222833
0.119067	-1.438187	1.051009	-1.280202	1.836159
-1.041588	0.318400	1.108142	3.414807	0.022161

-1.581547	2.368243	-1.230651	1.351662	-1.323080
-1.493846	-0.486470	-0.162774	0.452481	0.372186
-1.570053	1.065459	-0.507441	-0.709982	0.873252
-1.715788	1.505340	-1.036940	-1.523897	-1.331088

-1.577545	-3.272123	0.781748	0.320923	-1.652765
-0.770120	-1.432640	1.610934	-1.410051	1.012976
1.549749	-0.348732	-1.792113	0.121472	-1.693206
-1.463005	-0.055374	-1.122379	-0.617521	-1.821342

-1.755365	3.567013	1.935923	-2.000367	-1.933002
0.386278	1.014744	-0.659932	-1.790907	1.614744
0.297207	-1.239904	-1.452236	1.057482	0.248376
-0.307137	-1.891120	1.369759	1.585057	-0.942211

-1.811062	-2.164232	0.416019	2.710806	-2.140252
1.573129	1.405200	-1.575001	-0.027320	2.089371
-2.064396	2.302387	0.388581	1.876941	1.802193
1.203125	-0.760472	1.253378	1.043252	0.823439

-1.840077	1.357832	-1.935983	-1.357746	-2.253036
2.336195	-1.434920	1.371916	2.041451	2.357042
1.357873	-1.357838	2.135358	2.365288	-1.358703
2.284807	1.619227	-1.555616	-1.601145	2.217075

PROGRAM INTERRUPT() CLR PSW IS FF25007062026F84

SOLUTION OF THE DISPERSION MODEL EQUATION
 USING FINITE DIFFERENCE B.C.
 SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.000000	0.000000	0.000000	-0.000000	-0.000000
0.1	0.673440	0.734465	0.587788	0.444377	0.328489
0.2	0.938641	0.869128	0.773755	0.681632	0.587875
0.3	0.949713	0.910918	0.853745	0.790098	0.721713
0.4	0.972256	0.937949	0.897349	0.851164	0.800122
0.5	0.979855	0.954384	0.924215	0.889464	0.850402
0.6	0.984506	0.965233	0.942105	0.915271	0.884752
0.7	0.987886	0.972821	0.954695	0.933588	0.909442
0.8	0.990345	0.978358	0.968026	0.947171	0.927774
0.9	0.992193	0.982527	0.970899	0.957354	0.941754
1.0	0.993613	0.985737	0.976280	0.965292	0.952625

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.0	-0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.229340	0.154433	0.099715	0.062727	0.037249
0.2	0.438476	0.418702	0.332942	0.264646	0.206396
0.3	0.650674	0.579015	0.508626	0.441149	0.377917
0.4	0.745339	0.687982	0.629284	0.570454	0.512650
0.5	0.807699	0.761706	0.713950	0.664637	0.614867
0.6	0.851013	0.814379	0.775413	0.734721	0.692999
0.7	0.882502	0.853030	0.821403	0.788067	0.753568
0.8	0.906119	0.882312	0.856631	0.829413	0.801797
0.9	0.924290	0.904950	0.884072	0.861877	0.838725
1.0	0.933396	0.922698	0.905695	0.887596	0.868696

TIME	CONCENTRATIONS AT GRID POINTS				
	11	12	13	14	15
0.0	0.000000	0.000000	0.000000	-0.000000	-0.000000
0.1	0.001639	0.012184	0.006660	0.003541	0.001834
0.2	0.005089	0.011886	0.007929	0.004001	0.004590
0.3	0.010087	0.026766	0.022574	0.018192	0.014789
0.4	0.045088	0.040440	0.035487	0.031005	0.027008
0.5	0.050505	0.051738	0.047135	0.042824	0.038823
0.6	0.050449	0.050291	0.046816	0.043035	0.049470
0.7	0.071046	0.063368	0.048955	0.051598	0.058518
0.8	0.072181	0.074301	0.071429	0.066656	0.066729
0.9	0.014071	0.073100	0.076731	0.074449	0.072291
1.0	0.040271	0.062065	0.081022	0.079142	0.077370

TIME	CONCENTRATIONS AT GRID POINTS				
	16	17	18	19	20
0.0	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.000027	0.000458	0.000223	0.000111	0.000066
0.2	0.002542	0.022943	0.010334	0.012159	0.010099
0.3	0.011986	0.097724	0.080911	0.069484	0.063577
0.4	0.025404	0.056695	0.034172	0.038451	0.030191
0.5	0.035909	0.032428	0.030737	0.028406	0.027530
0.6	0.046274	0.043537	0.041343	0.039735	0.038952
0.7	0.055740	0.053349	0.051420	0.050051	0.049328
0.8	0.063726	0.061700	0.060066	0.058198	0.058276
0.9	0.070343	0.068688	0.067297	0.066239	0.065806
1.0	0.075705	0.074382	0.073208	0.072458	0.072032

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.048780	0.097560	0.146340	0.195120	0.243900
0.292680	0.341460	0.390240	0.439020	0.487800
0.536580	0.585360	0.634140	0.682920	0.731700
0.780480	0.829260	0.878040	0.926820	0.975600

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

18.9291	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

EIGENVALUES

1.813970	442.724889	4.933260	399.267672	156.553073
37.920738	263.181725	286.338728	129.018985	11.832931
335.825796	365.262639	78.350489	302.374733	22.888296
55.565293	154.551113	278.609363	212.185188	102.714559

EIGENVECTORS

-0.162001	0.000000	-0.296588	0.000011	0.249753
-0.336154	-0.095729	-0.045165	-0.274165	-0.333931
-0.002314	-0.000228	0.312474	-0.013293	-0.340410
0.326325	-0.221226	0.146019	-0.187361	0.294984

-0.178379	0.000001	0.312713	0.000053	0.303029
0.188600	-0.264321	-0.142474	-0.219741	0.317650
-0.003813	-0.000085	0.013036	-0.046632	0.267526
-0.092085	-0.351058	0.356377	-0.383268	0.120371

0.193347	0.000004	-0.312963	0.000136	-0.154921
0.050441	-0.380038	-0.258136	0.291360	-0.255394
-0.023223	-0.002975	-0.310216	-0.101664	-0.116281
-0.204153	-0.026892	0.371006	-0.225261	-0.343220

-0.206782	0.000014	0.298371	0.000597	-0.316460
-0.254154	-0.372681	-0.364525	0.148677	0.153589
-0.052162	-0.008034	0.267842	-0.185521	-0.062600
0.333884	0.330863	0.136447	0.158392	0.081107

0.218590	0.000051	-0.270579	0.001772	0.128994
0.327797	-0.178153	-0.401527	-0.321735	-0.045863
-0.104500	-0.010754	0.043299	-0.290417	0.216554
-0.216626	0.172070	-0.193401	0.343980	0.278184

-0.228689	0.000171	0.231657	0.004844	0.303640
-0.247387	0.110108	-0.305673	-0.029937	-0.069471
-0.185817	-0.044161	-0.300222	-0.382744	-0.305686
-0.046881	-0.257523	-0.335777	0.083002	-0.267792

..CONTD

0.237012	0.000538	-0.184021	0.012190	-0.147811
0.060086	0.318710	-0.071310	0.321959	0.171591
-0.289201	-0.289200	0.265725	-0.403456	0.311400
0.269025	-0.233059	-0.117333	-0.278465	-0.071827
-0.243512	0.001934	0.130190	0.028154	-0.270912
0.146214	0.263277	0.196823	-0.122216	-0.248801
-0.385119	-0.162135	0.005102	-0.295931	-0.238131
-0.309080	0.205990	0.228245	-0.225100	0.313907
0.240159	0.004120	-0.072782	0.059443	0.199899
-0.284714	-0.073731	0.315621	-0.246878	0.293508
-0.418900	-0.261194	-0.264075	-0.050701	0.100177
0.154616	0.247237	0.276441	0.174919	-0.187833
-0.250948	0.010265	0.014350	0.114072	0.207531
0.304442	-0.291166	0.171048	0.259235	-0.302613
-0.333456	-0.306530	0.291044	0.200821	0.041275
0.088047	-0.190608	-0.048093	0.276200	-0.142029
0.251868	0.023659	0.042785	0.197350	-0.261301
-0.205371	-0.160980	-0.127036	0.078627	0.277284
-0.116461	-0.433774	-0.080009	0.318105	-0.177338
-0.271285	-0.233134	-0.293306	-0.097470	0.303878
-0.250936	0.050275	-0.096419	0.304092	-0.101710
0.032169	-0.187701	-0.285868	-0.303033	-0.222358
0.153802	-0.404453	-0.187512	0.183415	0.269025
0.234982	0.200442	-0.087954	-0.285858	-0.149732
0.244186	0.002043	0.144719	0.409404	0.295955
0.147477	0.261231	-0.121707	0.136433	0.145409
0.320033	-0.241269	0.303298	-0.108324	-0.300816
-0.155732	0.194862	0.250582	0.059627	-0.155310
-0.243068	0.174436	-0.185157	0.485462	-0.042515
-0.263520	-0.018137	0.183415	0.198006	-0.055660
0.250054	0.023657	-0.190258	-0.236195	0.267903
-0.052408	-0.240430	0.163524	0.280889	0.290500

..CONTD

0.237448	0.280069	0.213572	0.415385	-0.268313
0.293148	-0.262939	0.245172	-0.282366	-0.037125
-0.022187	0.268370	-0.256381	-0.156071	-0.181222
0.241952	-0.127033	-0.202934	-0.057884	-0.155191

-0.229612	0.400432	-0.244173	0.229605	0.197589
-0.221157	-0.068218	-0.026980	0.241197	0.123658
-0.266710	0.233870	0.257174	0.148390	0.261950
-0.294451	0.272678	-0.196590	-0.269803	-0.123327

-0.220257	0.300059	0.259525	-0.249806	0.144795
0.077042	0.225434	-0.253210	0.239950	-0.195961
-0.240522	0.153447	-0.276339	0.263799	0.067636
0.201008	0.027486	0.172874	0.055572	0.288859

-0.204466	0.521103	-0.265520	-0.295683	-0.277677
0.087736	0.149046	-0.094937	-0.249567	0.247980
0.042242	-0.147802	0.111175	0.235371	-0.180404
-0.013957	-0.276822	0.203231	0.249086	-0.192517

0.197351	0.411513	0.262385	-0.353663	0.045380
-0.221075	-0.186729	0.207289	-0.208679	-0.275963
0.269332	-0.308161	0.121793	-0.235308	0.255864
-0.174768	0.094000	-0.165288	-0.134624	-0.065392

-0.184034	0.162460	-0.250638	-0.162943	0.238700
0.284240	-0.176149	0.165964	0.251343	0.273577
0.162960	-0.162351	-0.271908	-0.163200	-0.285271
0.273333	0.224590	-0.192288	-0.209044	0.252470

CHECK OF SIMILARITY TRANSFORMATION

75.432187	66.858915	-0.000000	-0.000000	-0.000000
0.000000	0.500000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000

66.858915	138.374294	60.968823	-0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000

..CONTD

-0.000000	67.568326	144.522675	73.278740	-0.000000
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	73.278740	150.675259	76.180248
-0.000000	-0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	76.180248	150.675259
79.281755	-0.000000	-0.000000	-0.000000	0.000000
-0.000000	0.000000	-0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	79.281755
162.976223	82.383262	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
82.383262	159.124604	85.476364	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	85.476364	175.272985	88.573669	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	88.573669	181.425569	91.666771
-0.000000	0.000000	0.000000	-0.000000	-0.000000
0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	91.666771	187.573950
94.764076	-0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000

..EDNFD

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	0.000000	-0.000000	14.754076
193.726523	97.557178	-0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	0.000000

0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
97.557178	193.726523	100.946077	-0.000000	0.000000
0.000000	0.000000	-0.000000	0.000000	0.000000

0.000000	0.0	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	100.946077	206.023295	104.039180	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000

-0.000000	0.000000	-0.000000	-0.000000	0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	-0.000000	104.039180	212.175879	107.128079
-0.000000	0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	107.128079	216.324260
110.212776	-0.000000	0.000000	-0.000000	-0.000000

-0.000000	-0.000000	-0.000000	0.000000	-0.000000
0.000000	0.000000	0.000000	0.000000	-0.000000
-0.000000	0.000000	0.000000	-0.000000	110.212776
224.475843	113.395878	-0.000000	0.000000	0.000000

0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	0.000000	0.000000	0.000000	-0.000000
113.395878	230.625224	116.394778	0.000000	0.000000

-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	116.394778	236.773505	119.477475	-0.000000

..CONTD

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	118.473475	242.925139	122.568374

-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	0.000000	-0.000000	122.568374	133.251344

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

1.813978	442.764639	-4.938267	399.287672	156.553073
37.921738	243.181725	286.338728	129.718925	11.832931
335.825796	365.043037	78.350469	309.374758	22.483296
57.555283	134.551117	238.609383	212.185133	102.714559

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.162001	-0.000000	0.296588	-0.000011	-0.244753
0.336154	0.035729	0.045165	0.274165	0.333931
0.082314	0.000228	-0.312424	0.013293	0.342410
-0.326325	0.221226	-0.146019	0.187381	-0.294984

-0.207811	0.000001	0.364311	0.000001	0.353023
0.219720	-0.313177	-0.165983	-0.255998	0.377062
-0.010530	-0.001148	0.015896	-0.054326	0.311668
-0.107280	-0.428632	0.415180	-0.446507	0.143232

-0.260632	-0.000000	0.421874	-0.000251	0.215574
-0.067995	0.523075	0.347967	-0.392753	0.344272
0.031204	0.004111	0.418171	0.137042	0.156746
0.275198	0.036250	-0.500116	0.303652	0.402660

-0.320573	0.000022	0.462565	0.000926	-0.491608
-0.394915	-0.577767	-0.555122	0.230339	0.247411
-0.080867	-0.012456	0.415236	-0.287614	-0.097049
0.517621	0.513972	0.211534	0.245554	0.126740

-0.367516	-0.000001	0.470682	-0.003141	-0.223680
-0.581100	0.315330	0.711827	0.570372	0.281306
0.185257	0.035720	-0.076781	0.514851	-0.383907
0.334735	-0.356541	0.351726	-0.609808	-0.493165

-0.461197	0.000344	0.467203	0.009789	0.612350
-0.493905	0.241221	-0.615450	-0.050360	-0.140103
-0.374738	-0.037059	-0.605458	-0.771879	-0.616477
-0.094545	-0.510346	-0.677181	0.177474	-0.540050

..CONTD

-0.541122	-0.721211	0.423138	-0.727830	0.437467
-0.137168	-0.722187	0.162808	-0.735065	-0.391760
0.662523	-0.233396	-0.608360	0.421137	-0.712958
-0.614211	0.534215	0.267283	0.555763	0.163988

-0.626604	0.703946	0.335076	0.072447	-0.697112
0.376227	0.692268	0.506466	-0.314487	-0.640215
-0.990987	-0.417208	0.015701	-0.761490	-0.612754
-0.795325	0.530054	0.587320	-0.579229	0.807745

-0.716709	-0.711999	0.210200	-0.171673	-0.577329
0.822384	0.212044	-0.911544	0.713009	-0.847683
1.209825	0.764355	0.762675	0.175311	-0.315313
-0.446547	-0.714219	-0.793389	-0.505184	0.542481

-0.810317	0.733145	0.046271	0.368340	0.673118
0.983042	-0.940173	0.552312	0.837069	-0.977137
-1.076730	-1.103544	0.939782	0.648452	0.133278
0.284303	-0.616472	-0.155292	0.891851	-0.458612

-0.905995	-0.785105	-0.153902	-0.709889	0.939925
0.733742	0.579081	0.456961	-0.282931	-0.997418
0.416922	1.560329	0.287799	-1.144256	0.637904
0.975838	0.338008	1.055052	0.350608	-1.111066

-1.002112	0.300774	-0.335049	1.214393	-0.406179
0.128465	0.663714	-1.141514	-1.210161	-0.837988
0.614209	-1.615132	-0.743331	0.732470	-1.076749
1.173009	0.824427	-0.351244	-1.141565	-0.597955

-1.096835	-0.453223	-0.639569	-1.809321	-1.312361
-0.651761	-1.154488	0.537873	-0.603172	-0.642621
-1.414255	1.066262	-1.340397	0.478727	1.329428
0.688506	-0.663791	-1.107422	-0.263517	0.686376

-1.183172	0.452222	-0.907738	2.269687	-0.207310
-1.314137	-0.093607	0.894366	0.941136	-0.271410
1.219312	0.115857	-0.927737	-1.325544	1.375348
-0.224316	-1.173677	0.793838	1.309469	1.660422

..CONT

-1.273843	-1.302536	-1.177961	-2.228493	1.428769
-1.583427	1.410102	-1.315326	1.514856	-0.199171
0.113032	-1.433168	0.305160	0.537307	0.972240
-1.298748	0.531544	1.036720	0.310540	0.832586

-1.351705	2.860248	-1.437420	1.351662	1.121976
-1.301927	-0.519918	-0.153830	0.242522	0.727904
-1.570093	1.065760	1.513955	0.673613	0.358805
-1.733401	1.695231	-1.157303	-1.588302	-0.755440

-1.419223	-3.222129	-1.672247	0.320923	-0.952988
-0.494419	-1.452072	1.631559	-1.546171	1.262676
1.543801	-0.988733	1.780591	-1.699727	-0.437103
-1.295198	-0.177104	-1.113911	-0.551385	-1.861262

-1.473761	3.567013	-1.863146	-2.080357	-1.953577
0.617295	1.048561	-0.667959	-1.755904	1.744733
0.297207	-1.539065	0.782204	0.248665	-1.269286
-0.098200	-1.044147	1.429891	1.752516	-1.354512

-1.512712	-0.154292	-2.011207	2.710866	-0.347840
1.694558	1.431299	-1.583889	0.066526	2.115286
-2.064456	0.362784	-0.933555	1.803660	-1.958885
1.339610	-0.720517	1.263947	1.031906	0.501237

-1.533518	1.357832	-2.088514	-1.357746	1.939038
2.368513	-1.467814	1.382348	2.094394	2.321326
1.357915	-1.357832	-2.265752	-1.359917	-2.377106
2.327623	1.371460	-1.602295	-1.741921	2.187113

PROGRAM INTERRUPT () CLR PSW IS FF25000062020F34

SOLUTION OF THE DISPERSION MODEL EQUATION
 USING DANCKWERTS B.C.
 SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS					
TIME	1	2	3	4	5
0.0	0.000000	-0.000000	0.000000	-0.000000	0.000000
0.1	0.520285	0.408690	0.378197	0.223190	0.155321
0.2	0.573406	0.597243	0.515506	0.436527	0.362422
0.3	0.787053	0.706162	0.642128	0.576722	0.511523
0.4	0.824064	0.777150	0.726523	0.673265	0.618323
0.5	0.867427	0.826501	0.785990	0.742557	0.696753
0.6	0.891822	0.862280	0.829497	0.793888	0.755758
0.7	0.912952	0.889024	0.862239	0.832882	0.801097
0.8	0.929082	0.909497	0.887439	0.863112	0.836563
0.9	0.941645	0.925471	0.907135	0.886937	0.864712
1.0	0.951574	0.938127	0.922353	0.905965	0.887313

CONCENTRATIONS AT GRID POINTS					
TIME	6	7	8	9	10
0.0	-0.000000	0.000000	-0.000000	0.000000	-0.000000
0.1	0.104006	0.067112	0.041796	0.025155	0.014673
0.2	0.296171	0.235912	0.185113	0.142679	0.108087
0.3	0.443194	0.387764	0.331530	0.280123	0.234003
0.4	0.552330	0.507790	0.454147	0.402713	0.354173
0.5	0.649358	0.601113	0.552769	0.505043	0.458618
0.6	0.715651	0.674104	0.631702	0.589036	0.546729
0.7	0.767282	0.731826	0.695184	0.657344	0.620343
0.8	0.808090	0.777981	0.745599	0.714339	0.681659
0.9	0.840743	0.815247	0.788516	0.760877	0.732730
1.0	0.857132	0.845573	0.828880	0.799324	0.775250

CONCENTRATIONS AT GRID POINTS					
TIME	11	12	13	14	15
0.0	0.000000	-0.000000	0.000000	0.000000	-0.000000
0.1	0.004209	0.004561	0.002439	0.001271	0.000646
0.2	0.008524	0.009028	0.004260	0.002302	0.001263
0.3	0.012839	0.013817	0.007882	0.004587	0.002173
0.4	0.017154	0.018686	0.011371	0.007269	0.004469
0.5	0.021469	0.023783	0.014283	0.010946	0.007461
0.6	0.025784	0.029547	0.017614	0.014299	0.010350
0.7	0.030099	0.034646	0.021147	0.017910	0.014931
0.8	0.034414	0.039332	0.025875	0.021646	0.019239
0.9	0.038729	0.043496	0.030907	0.025337	0.023922
1.0	0.043044	0.047641	0.035339	0.028959	0.028053

CONCENTRATIONS AT GRID POINTS					
TIME	16	17	18	19	20
0.0	0.000000	-0.000000	-0.000000	0.000000	-0.000000
0.1	0.000021	0.000156	0.000075	0.000037	0.000021
0.2	0.000043	0.000193	0.000111	0.000094	0.000043
0.3	0.000064	0.000238	0.000148	0.000104	0.000064
0.4	0.000086	0.000283	0.000186	0.000133	0.000086
0.5	0.000107	0.000320	0.000225	0.000164	0.000107
0.6	0.000129	0.000357	0.000263	0.000198	0.000129
0.7	0.000150	0.000396	0.000301	0.000237	0.000150
0.8	0.000171	0.000433	0.000330	0.000264	0.000171
0.9	0.000193	0.000470	0.000364	0.000295	0.000193
1.0	0.000214	0.000507	0.000398	0.000326	0.000214


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C          PROGRAM FOR INTERPOLATION
C  INTERPOLATE THE VALUES OF CONCENTRATION
C  CORRESPONDING TO ONE GRID FROM THOSE
C  OF A HIGHER POINT GRID
C  N= THE NUMBER OF GRID POINTS ( THE VALUES
C  TO BE INTERPOLATED)
C  NN= THE NUMBER OF GRID POINTS ( GREATER THAN
C  ABOVE)
C  NT= THE TOTAL NUMBER OF TIMES
C  GRIDX=THE DIMENSIONLESS DISTANCES OF GRID POINTS
C  (CORRESPONDING TO THE VALUES TO BE INTERPOLATED)
C  GRIDN=THE DIMENSIONLESS DISTANCES OF GRID POINTS
C  (CORRESPONDING TO THE HIGHER POINT GRID)
REAL GRIDX(10),GRIDN(20),TIME(15),CONC(15,10)
1,CEVR(15,20),WORK(300)
REAL CINTP(15,10),ERROR(15,10),X,F(300),ARG(20)
1,Z(20),Y,YY(20),VAL(300)
INTEGER I,J,N,NN,NT
READ(5,1)  N,NN,NT
READ(5,2)  (TIME(J),J=1,NT)
DO 3 J=1,NT
READ(5,6)  (CEVR(J,K),K=1,NN)
3 CONTINUE
DO 5 J=1,NT
READ(5,6)  (CONC(J,K),K=1,N)
5 CONTINUE
READ(5,13) (GRIDX(J),J=1,N)
READ(5,13) (GRIDN(J),J=1,NN)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,4,2)
WRITE(6,264)
CALL LINECT(LINES,3,2)
WRITE(6,265) (GRIDX(I),I=1,N)
WRITE(6,222)
WRITE(6,266)
CALL LINECT(LINES,3,2)
WRITE(6,265) (GRIDN(I),I=1,NN)
WRITE(6,223)
WRITE(6,225)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,247)
WRITE(6,248)
DO 7 J=1,NT
7 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)

```



```

WRITE(6,246)
WRITE(6,249)
DO 8 J=1,NT
8 WRITE(6,251) TIME(J), (CEVR(J,K),K=6,10)
WRITE(6,220)
WRITE(6,246)
WRITE(6,259)
DO 15 J=1,NT
15 WRITE(6,251) TIME(J), (CEVR(J,K),K=11,15)
WRITE(6,223)
WRITE(6,246)
WRITE(6,258)
DO 16 J=1,NT
16 WRITE(6,251) TIME(J), (CEVR(J,K),K=16,20)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,3,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,250)
WRITE(6,248)
DO 9 J=1,NT
9 WRITE(6,251) TIME(J), (CONC(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)
WRITE(6,249)
DO 17 J=1,NT
17 WRITE(6,251) TIME(J), (CONC(J,K),K=6,10)
DO 14 JJ=1,NN
Z(JJ)=GRIDN(JJ)
14 CONTINUE
C
C THE TABLE OF Z VS F READY FOR ONE VALUE OF TIME
C
C
C ORDER THE TABLE USING S.S.P
C
IROW=20
ICOL=1
NDIM=20
DO 19 J=1,NT
DO 19 I=1,N
X=GRIDX(I)
DO 31 JJ=1,NN
F(JJ)=CEVR(J,JJ)
31 CONTINUE
CALL ATSG(X,Z,F,WORK,IROW,ICOL,ARG,VAL,NDIM)
EPS=0.00001
CALL ALI(X,ARG,VAL,Y,NDIM,EPS,IER)

```



```

      YY(I)=Y
      CINTP(J,I)=YY(I)
19  CONTINUE
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,260)
      WRITE(6,248)
      DO 20 J=1,NT
20  WRITE(6,251)  TIME(J),(CINTP(J,K),K=1,5)
      WRITE(6,223)
      WRITE(6,249)
      DO 30 J=1,NT
30  WRITE(6,251)  TIME(J), (CINTP(J,K),K=6,10)
      DO 27 J=1,NT
      DO 27 K=1,N
27  ERROR(J,K)=CINTP(J,K)-CONC(J,K)
      WRITE(6,223)
      WRITE(6,255)
      WRITE(6,223)
      WRITE(6,248)
      DO 28 J=1,NT
28  WRITE(6,251)  TIME(J), (ERROR(J,K),K=1,5)
      WRITE(6,223)
      WRITE(6,255)
      WRITE(6,223)
      WRITE(6,249)
      DO 29 J=1,NT
29  WRITE(6,251)  TIME(J), (ERROR(J,K),K=6,10)

```

C FORMAT STATEMENTS

```

 1  FORMAT(1X,3I3)
 2  FORMAT(10F7.3)
 6  FORMAT(5F16.6)
13  FORMAT(10F8.5)
220 FORMAT(1H2)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,19HUSING ORDINARY B.C.)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
247 FORMAT(1H,40X,17HTWENTY POINT GRID)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
      12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
      18X,2H 9, 8X, 2H10)
250 FORMAT(1H,40X,14HTEN POINT GRID)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
255 FORMAT(1H,30X,18H ASSOCIATED ERRORS)
258 FORMAT(1H,15X,5H TIME,9X,2H16,8X,2H17,8X,2H18,

```



```
18X,2H19,8X,2H20)  
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,  
18X,2H14,8X,2H15)  
260 FORMAT(1H,30X,20H INTERPOLATED VALUES)  
264 FORMAT(1H,25X,27HGRID POINTS(TEN POINT GRID))  
265 FORMAT(1H,10X,5F10.6)  
266 FORMAT(1H,25X,30HGRID POINTS(TWENTY POINT GRID))  
STOP  
END
```


GRID POINTS(TEN POINT GRID)

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

GRID POINTS(TWENTY POINT GRID)

0.048780	0.097560	0.146340	0.195120	0.243900
0.292680	0.341460	0.390240	0.439020	0.487800
0.536580	0.585360	0.634140	0.682920	0.731700
0.780480	0.829260	0.878040	0.926820	0.975600

SOLUTION OF THE DISPERSION MODELEQUATION
USING ORDINARY B.C.

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS
TWENTY POINT GRID

TIME	1	2	3	4	5
0.1	0.876490	0.734465	0.587786	0.449377	0.328480
0.2	0.936641	0.869128	0.773755	0.681632	0.587875
0.3	0.960013	0.910918	0.853745	0.790098	0.721713
0.4	0.972266	0.937949	0.897349	0.851164	0.800122
0.5	0.979655	0.954384	0.924215	0.889464	0.850402
0.6	0.984506	0.965233	0.942105	0.915271	0.884782
0.7	0.987886	0.972281	0.954695	0.933588	0.909422
0.8	0.990345	0.978358	0.963926	0.947101	0.927774
0.9	0.992193	0.982587	0.970399	0.957354	0.941759
1.0	0.993613	0.985737	0.976280	0.965290	0.952625

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	0.229940	0.154433	0.099715	0.062027	0.037249
0.2	0.496476	0.410702	0.332942	0.264646	0.206396
0.3	0.650676	0.579015	0.508625	0.441149	0.377917
0.4	0.745339	0.687982	0.629284	0.570454	0.512650
0.5	0.807655	0.761906	0.713950	0.664637	0.614867
0.6	0.851013	0.814379	0.775413	0.734721	0.692999
0.7	0.882502	0.853030	0.821403	0.788067	0.753568
0.8	0.906119	0.882312	0.856631	0.829413	0.801097
0.9	0.924250	0.904950	0.884072	0.861377	0.838725
1.0	0.938398	0.922698	0.905695	0.887596	0.868696

CONCENTRATIONS AT GRID POINTS					
TIME	11	12	13	14	15
0.1	0.021639	0.012184	0.006660	0.003541	0.001834
0.2	0.158039	0.113886	0.087929	0.064001	0.045908
0.3	0.319887	0.267666	0.221574	0.181692	0.147897
0.4	0.455888	0.404040	0.354876	0.310051	0.270089
0.5	0.555505	0.517385	0.471353	0.428242	0.388823
0.6	0.650949	0.609291	0.568816	0.530351	0.494700
0.7	0.713469	0.683368	0.648955	0.615981	0.585185
0.8	0.772131	0.743001	0.714293	0.686560	0.660729
0.9	0.814971	0.791005	0.767314	0.744449	0.722941
1.0	0.849279	0.829654	0.810222	0.791442	0.773750

CONCENTRATIONS AT GRID POINTS					
TIME	16	17	18	19	20
0.1	0.000927	0.000458	0.000223	0.000111	0.000066
0.2	0.032542	0.022943	0.016334	0.012159	0.010099
0.3	0.119986	0.097724	0.080911	0.069484	0.063577
0.4	0.235484	0.206695	0.184172	0.166451	0.160191
0.5	0.353905	0.324285	0.300737	0.284106	0.275310
0.6	0.462744	0.435373	0.413435	0.397851	0.389582
0.7	0.557405	0.533490	0.514233	0.500517	0.493228
0.8	0.637260	0.617005	0.600660	0.586989	0.582786
0.9	0.703437	0.686588	0.672972	0.663239	0.658068
1.0	0.757695	0.743825	0.732608	0.724534	0.720324

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS TEN POINT GRID

TIME	1	2	3	4	5
0.1	0.736693	0.460556	0.248719	0.118506	0.050751
0.2	0.362382	0.687305	0.507696	0.348425	0.223531
0.3	0.913151	0.795302	0.659648	0.521591	0.393844
0.4	0.940129	0.855958	0.753387	0.541056	0.527629
0.5	0.950523	0.894039	0.815227	0.725076	0.629207
0.6	0.967345	0.919715	0.858301	0.786132	0.706873
0.7	0.974915	0.937947	0.889604	0.831852	0.767112
0.8	0.980440	0.951404	0.913100	0.866906	0.814437
0.9	0.984602	0.961624	0.931160	0.894253	0.851978
1.0	0.987811	0.969546	0.945277	0.915851	0.881960

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	0.019846	0.007185	0.002429	0.000786	0.000281
0.2	0.134938	0.077168	0.042147	0.022857	0.014034
0.3	0.285049	0.198764	0.134990	0.093113	0.071142
0.4	0.421375	0.328197	0.252301	0.196583	0.168585
0.5	0.534376	0.446396	0.370882	0.315692	0.283727
0.6	0.625905	0.548224	0.479472	0.428689	0.398453
0.7	0.699697	0.633636	0.574006	0.530057	0.503204
0.8	0.759191	0.704277	0.654002	0.617378	0.594358
0.9	0.807203	0.762226	0.720570	0.690831	0.671502
1.0	0.845984	0.809529	0.775401	0.751739	0.735707

INTERPOLATED VALUES					
TIME	1	2	3	4	5
0.1	0.741446	0.461903	0.242607	0.108693	0.042180
0.2	0.864021	0.590528	0.509239	0.347038	0.219346
0.3	0.913447	0.796385	0.660894	0.521838	0.392512
0.4	0.939728	0.855779	0.753340	0.640497	0.526246
0.5	0.955699	0.892959	0.813954	0.723203	0.626697
0.6	0.966238	0.917980	0.856015	0.782978	0.702976
0.7	0.973046	0.935734	0.886503	0.827566	0.761847
0.8	0.978983	0.948807	0.909343	0.861644	0.807906
0.9	0.983092	0.958726	0.926859	0.888152	0.844297
1.0	0.986147	0.966405	0.940520	0.909020	0.873247

TIME	6	7	8	9	10
0.1	0.014393	0.004381	0.001204	0.000302	0.000079
0.2	0.129176	0.071262	0.037135	0.018838	0.010826
0.3	0.281952	0.194287	0.129928	0.087444	0.065689
0.4	0.418776	0.324459	0.247989	0.193014	0.163142
0.5	0.530940	0.442223	0.366609	0.310021	0.278455
0.6	0.621093	0.542885	0.474410	0.422102	0.392541
0.7	0.693344	0.626755	0.567563	0.521853	0.495835
0.8	0.751294	0.695625	0.645852	0.607129	0.585001
0.9	0.797838	0.751938	0.710578	0.678362	0.659916
1.0	0.835252	0.797596	0.763573	0.737050	0.721348

ASSOCIATED ERRORS

TIME	1	2	3	4	5
0.1	0.004753	0.001347	-0.006112	-0.009613	-0.008571
0.2	0.001639	0.002723	0.001543	-0.001387	-0.004185
0.3	0.000296	0.001083	0.001246	0.000247	-0.001332
0.4	-0.000401	-0.000179	-0.000047	-0.000559	-0.001383
0.5	-0.000824	-0.001080	-0.001273	-0.001873	-0.002510
0.6	-0.001107	-0.001735	-0.002286	-0.003155	-0.003897
0.7	-0.001869	-0.002213	-0.003101	-0.004236	-0.005265
0.8	-0.001457	-0.002597	-0.003757	-0.005262	-0.006531
0.9	-0.001510	-0.002898	-0.004301	-0.006101	-0.007681
1.0	-0.001664	-0.003141	-0.004757	-0.006831	-0.008713

ASSOCIATED ERRORS

TIME	6	7	8	9	10
0.1	-0.005448	-0.002804	-0.001225	-0.000484	-0.000202
0.2	-0.005762	-0.005906	-0.005012	-0.004019	-0.003208
0.3	-0.003097	-0.004477	-0.005062	-0.005668	-0.005453
0.4	-0.002599	-0.003738	-0.004312	-0.005569	-0.005443
0.5	-0.003436	-0.004173	-0.004273	-0.005671	-0.005272
0.6	-0.004812	-0.005339	-0.005062	-0.006587	-0.005912
0.7	-0.006353	-0.006881	-0.006443	-0.008204	-0.007369
0.8	-0.007396	-0.008652	-0.008150	-0.010249	-0.009357
0.9	-0.009365	-0.010288	-0.009992	-0.012469	-0.011586
1.0	-0.010732	-0.011932	-0.011828	-0.014639	-0.013859


```

      PROGRAM FOR INTERPOLATION
      INTERPOLATE THE VALUES OF CONCENTRATION
      CORRESPONDING TO THE GRID FROM THOSE
      OF A HIGHER POINT GRID
      N= THE NUMBER OF GRID POINTS ( THE VALUES
      TO BE INTERPOLATED)
      NN= THE NUMBER OF GRID POINTS ( GREATER THAN
      ABOVE)
      NT= THE TOTAL NUMBER OF TIMES
      X= THE DIMENSIONLESS DISTANCES OF THE GRID
      POINTS CORRESPONDING TO THE VALUES TO BE
      INTERPOLATED)
      XX= THE DIMENSIONLESS DISTANCES OF THE GRID
      POINTS (CORRESPONDING TO THE HIGHER POINT GRID)
      REAL X(10),XX(30),TIME(15),CONC(15,10),
1 CEVR(15,20),CGRID(15,10)
      REAL CINTP(15,10),ERROR(15,10)
      INTEGER I,J,N,NN,NT
      READ(5,1) N,NN,NT
      READ(5,2) (TIME(J),J=1,NT)
      DO 3 J=1,NT
      READ(5,6) (CEVR(J,K),K=1,NN)
3 CONTINUE
      DO 5 J=1,NT
      READ(5,6) (CONC(J,K),K=1,N)
5 CONTINUE
      READ(5,13) (X(J),J=1,N)
      READ(5,13) (XX(J),J=1,NN)
      WRITE(6,220)
      LINES=10
      CALL LINECT(LINES,4,2)
      WRITE(6,261)
      CALL LINECT(LINES,3,2)
      WRITE(6,262) (X(I),I=1,N)
      WRITE(6,222)
      WRITE(6,263)
      CALL LINECT(LINES,3,2)
      WRITE(6,262) (XX(I),I=1,NN)
      WRITE(6,223)
      WRITE(6,225)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,245)
      WRITE(6,223)
      WRITE(6,246)
      WRITE(6,247)
      WRITE(6,248)
      DO 7 J=1,NT
7 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
      WRITE(6,223)

```



```

WRITE(6,245)
WRITE(6,249)
DO 8 J=1,NT
8 WRITE(6,251) TIME(J),(CFVR(J,K),K=6,11)
WRITE(6,220)
WRITE(6,245)
WRITE(6,259)
DO 15 J=1,NT
15 WRITE(6,251) TIME(J),(CEVR(J,K),K=11,15)
WRITE(6,223)
WRITE(6,246)
WRITE(6,253)
DO 16 J=1,NT
16 WRITE(6,251) TIME(J),(CEVR(J,K),K=16,20)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,3,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,250)
WRITE(6,248)
DO 9 J=1,NT
9 WRITE(6,251) TIME(J),(CUNC(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)
WRITE(6,249)
DO 17 J=1,NT
17 WRITE(6,251) TIME(J),(CUNC(J,K),K=6,10)
CALL CALC(20,N,NT,CEVR,1,X,TIME,CINTP,XX)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,260)
WRITE(6,248)
DO 19 J=1,NT
19 WRITE(6,251) TIME(J),(CINTP(J,K),K=1,5)
WRITE(6,223)
WRITE(6,249)
DO 30 J=1,NT
30 WRITE(6,251) TIME(J),(CINTP(J,K),K=6,10)
DO 27 J=1,NT
DO 27 K=1,N
27 ERROR(J,K)=CINTP(J,K)-CUNC(J,K)
WRITE(6,220)
WRITE(6,255)
WRITE(6,223)
WRITE(6,243)
DO 11 J=1,NT
11 WRITE(6,251) TIME(J),(ERROR(J,K),K=1,5)

```



```

WRITE(6,223)
WRITE(6,255)
WRITE(6,223)
WRITE(6,249)
DO 29 J=1,IT
29 WRITE(6,251) TIME(J), (ERROR(J,K),K=6,10)
      FORMAT STATEMENTS
1 FORMAT(1X,3I3)
2 FORMAT(10F7.3)
6 FORMAT(5F16.6)
13 FORMAT(10F3.5)
220 FORMAT(1H2)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
      18HEQUATION/20X,21HUSING DANCKWERTS B.C.)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
247 FORMAT(1H,40X,17HTWENTY POINT GRID)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 3X,
      12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
      18X,2H 9, 8X, 2H10)
250 FORMAT(1H,40X,14HTEN POINT GRID)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
255 FORMAT(1H,30X,18H ASSOCIATED ERRORS)
258 FORMAT(1H,15X,5H TIME,9X,2H16,8X,2H17,8X,2H18,
      18X,2H19,8X,2H20)
259 FORMAT(1H,15X,5H TIME,5X,2H11,9X,2H12,8X,2H13,
      18X,2H14,8X,2H15)
260 FORMAT(1H,30X,20H INTERPOLATED VALUES)
261 FORMAT(1H,25X,27HGRID POINTS(TEN POINT GRID))
262 FORMAT(1H,10X,5F10.6)
263 FORMAT(1H,25X,30HGRID POINTS(TWENTY POINT GRID))
STOP
END

```


GRID POINTS(TEN POINT GRID)

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

GRID POINTS(TWENTY POINT GRID)

0.048780	0.097560	0.146340	0.195120	0.243900
0.292680	0.341460	0.390240	0.439020	0.487800
0.536580	0.585360	0.634140	0.682920	0.731700
0.780480	0.829260	0.878040	0.926820	0.975600

SOLUTION OF THE DISPERSION MODELEQUATION
USING DANCKWERTS B.C.

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS
TWENTY POINT GRID

TIME	1	2	3	4	5
0.1	0.520205	0.408690	0.308197	0.223190	0.155321
0.2	0.678406	0.597243	0.515606	0.436527	0.362422
0.3	0.767053	0.706162	0.642128	0.576722	0.511523
0.4	0.824084	0.777150	0.726523	0.673265	0.618328
0.5	0.863437	0.826501	0.785990	0.742557	0.696753
0.6	0.891822	0.862280	0.829497	0.793888	0.755758
0.7	0.912958	0.889024	0.862239	0.832882	0.801097
0.8	0.929089	0.909497	0.887439	0.863112	0.836563
0.9	0.941645	0.925471	0.907185	0.886937	0.864712
1.0	0.951574	0.938127	0.922883	0.905965	0.887318

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	0.104006	0.067112	0.041796	0.025165	0.014673
0.2	0.295171	0.235912	0.185113	0.142679	0.108087
0.3	0.448104	0.387764	0.331530	0.280128	0.234003
0.4	0.562830	0.507790	0.454147	0.402713	0.354173
0.5	0.649358	0.601113	0.552769	0.505043	0.458618
0.6	0.715561	0.674104	0.631702	0.589038	0.546729
0.7	0.767282	0.731826	0.695184	0.657844	0.620343
0.8	0.808090	0.777981	0.746599	0.714339	0.681669
0.9	0.840743	0.815247	0.788516	0.760877	0.732730
1.0	0.867132	0.845573	0.822880	0.799324	0.775250

TIME	CONCENTRATIONS AT GRID POINTS				
	11	12	13	14	15
0.1	0.008299	0.004561	0.002439	0.001271	0.000646
0.2	0.080524	0.059028	0.042604	0.030302	0.021263
0.3	0.193319	0.158017	0.127382	0.102587	0.081735
0.4	0.309042	0.267686	0.230371	0.197269	0.168469
0.5	0.414091	0.371983	0.332783	0.296946	0.264861
0.6	0.505352	0.465457	0.427614	0.392399	0.360350
0.7	0.583203	0.546946	0.512147	0.479410	0.449315
0.8	0.649043	0.616932	0.585875	0.556456	0.529239
0.9	0.704466	0.676496	0.649307	0.623437	0.599402
1.0	0.750988	0.726891	0.703388	0.680959	0.660063

TIME	CONCENTRATIONS AT GRID POINTS				
	16	17	18	19	20
0.1	0.000321	0.000156	0.000075	0.000037	0.000021
0.2	0.014758	0.010193	0.007111	0.005194	0.004257
0.3	0.064928	0.051798	0.042048	0.035504	0.032146
0.4	0.144048	0.124083	0.108678	0.098033	0.092473
0.5	0.236941	0.213600	0.195255	0.182404	0.175639
0.6	0.332056	0.308114	0.289108	0.275698	0.268609
0.7	0.422519	0.399686	0.381455	0.368537	0.361695
0.8	0.504876	0.484033	0.467330	0.455464	0.449173
0.9	0.577818	0.559307	0.544440	0.533860	0.528249
1.0	0.641260	0.625115	0.612128	0.602876	0.597969

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS
TEN POINT GRID

TIME	1	2	3	4	5
0.1	0.430437	0.249537	0.127341	0.058121	0.024076
0.2	0.604319	0.451520	0.314881	0.205828	0.126674
0.3	0.707003	0.584317	0.461551	0.394038	0.253152
0.4	0.775370	0.675795	0.571764	0.467913	0.371284
0.5	0.823811	0.744029	0.655500	0.563679	0.473448
0.6	0.859530	0.794473	0.720226	0.640712	0.559699
0.7	0.886636	0.833253	0.771095	0.703052	0.631994
0.8	0.907670	0.863650	0.811655	0.753878	0.692497
0.9	0.924285	0.887854	0.844384	0.795600	0.743144
1.0	0.937596	0.907368	0.871050	0.830042	0.785572

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10
0.1	0.009171	0.003251	0.001080	0.000344	0.000121
0.2	0.073799	0.040934	0.021766	0.011519	0.008928
0.3	0.176695	0.119232	0.078560	0.052683	0.039884
0.4	0.286531	0.216108	0.161141	0.123341	0.102668
0.5	0.389645	0.315797	0.254903	0.211463	0.186821
0.6	0.481683	0.410360	0.349545	0.305454	0.279730
0.7	0.561934	0.496312	0.439112	0.397463	0.372655
0.8	0.631035	0.572492	0.520656	0.483053	0.460147
0.9	0.690092	0.638934	0.593085	0.560163	0.539612
1.0	0.740318	0.696262	0.656373	0.628190	0.610095

INTERPOLATED VALUES

TIME	1	2	3	4	5
0.1	0.413744	0.230564	0.110396	0.045855	0.016719
0.2	0.601113	0.443873	0.304304	0.194130	0.115645
0.3	0.709129	0.582959	0.456994	0.341878	0.244484
0.4	0.779465	0.678418	0.570744	0.464206	0.365426
0.5	0.828338	0.746799	0.656189	0.561940	0.469508
0.6	0.863758	0.797388	0.721392	0.639809	0.556727
0.7	0.890226	0.835781	0.772215	0.702223	0.629247
0.8	0.910484	0.865522	0.812259	0.752648	0.689450
0.9	0.926287	0.883947	0.844261	0.793681	0.739448
1.0	0.938807	0.907647	0.870099	0.827271	0.781003

TIME	6	7	8	9	10
0.1	0.005418	0.001579	0.000418	0.000102	0.000026
0.2	0.064601	0.033993	0.016972	0.008269	0.004580
0.3	0.167554	0.110495	0.070869	0.045819	0.033346
0.4	0.279087	0.207816	0.152819	0.114701	0.094483
0.5	0.383724	0.308479	0.247047	0.202464	0.178097
0.6	0.476657	0.403798	0.342340	0.296597	0.271192
0.7	0.557168	0.490044	0.432283	0.388649	0.364191
0.8	0.626011	0.566033	0.513766	0.473928	0.451469
0.9	0.684419	0.631871	0.585701	0.550316	0.530298
1.0	0.733725	0.688278	0.648131	0.617263	0.599761

ASSOCIATED ERRORS

TIME	1	2	3	4	5
0.1	-0.016693	-0.018973	-0.016945	-0.012266	-0.007357
0.2	-0.003206	-0.007647	-0.010577	-0.011698	-0.011029
0.3	0.002126	-0.001358	-0.004557	-0.052160	-0.008668
0.4	0.004095	0.001623	-0.001020	-0.003707	-0.005858
0.5	0.004527	0.002770	0.000689	-0.001739	-0.003940
0.6	0.004228	0.002915	0.001166	-0.000903	-0.002972
0.7	0.003590	0.002528	0.001120	-0.000829	-0.002747
0.8	0.002814	0.001872	0.000604	-0.001230	-0.003047
0.9	0.002002	0.001093	-0.000123	-0.001919	-0.003696
1.0	0.001211	0.000279	-0.000951	-0.002771	-0.004569

ASSOCIATED ERRORS

TIME	6	7	8	9	10
0.1	-0.003753	-0.001672	-0.000662	-0.000242	-0.000095
0.2	-0.009197	-0.006941	-0.004794	-0.003250	-0.004348
0.3	-0.009141	-0.008737	-0.007691	-0.006864	-0.006538
0.4	-0.007444	-0.003292	-0.008322	-0.008640	-0.008185
0.5	-0.005921	-0.007318	-0.007856	-0.008949	-0.008724
0.6	-0.005026	-0.006562	-0.007205	-0.008857	-0.008538
0.7	-0.004766	-0.006268	-0.006829	-0.008814	-0.008464
0.8	-0.005024	-0.006459	-0.006890	-0.009125	-0.008677
0.9	-0.005673	-0.007063	-0.007384	-0.009847	-0.009314
1.0	-0.006593	-0.007984	-0.008242	-0.010927	-0.010334

APPENDIX E

ONE DIMENSIONAL HOMOGENEOUS CASE

(Using Higher Order Correct Formulations)

The partial differential equation describing this problem is

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z} .$$

The boundary conditions are:

- (i) at $z = 0$, $c = 1$
at $z = 1$, $\frac{\partial c}{\partial z} = 0$
- (ii) at $z = 0$, $c_{in}(\theta) = c_{z \rightarrow 0^+} - \alpha \left(\frac{\partial c}{\partial z} \right)_{z \rightarrow 0^+}$
at $z = 1$, $\frac{\partial c}{\partial z} = 0$.

(The higher order correct finite difference formulations as suggested by H.S. Price are shown in Figure IV-a).

Semi Analytical Solution A five point and a ten point grid are used to get the solution to the problem. $0 \leq z \leq 1$. The grid spacing is as shown in Figure IV-b).

Interpolated Values The results of the five point grid are derived from those of the ten point grid using interpolation to get a brief idea regarding the accuracy of the solution.

Deviations (Errors)

= Interpolated value - the value given by semi analytical solution


```

C      SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C      DIMENSIONAL HOMOGENEOUS CASE
C      USING HIGHER ORDER CORRECT MONOTONE TYPE
C      APPROXIMATIONS
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
C      REAL MATRIX(5,5),B(5,5),VECTOR(5,5),E(5),XX(5),
1X1(5),W(5,5),X(5),VAR(5),CI(5),C1(5),CEVR(15,5),
2TIME(15),D,VICTOR(5,5),X2(5),X3(5),A
C      READ THE DATA
      READ( 5,1)  N,NT
      READ(5,5)  ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 )  (X(J),J=1,N)
      READ( 5,2 )  (CI(J),J=1,N)
      READ(5,2)  (C1(J),J=1,N)
      READ(5,3)  (TIME(J), J=1,NT)
      READ(5,4) DX
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,220)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,223)
      WRITE(6,231)
      CALL LINECT(LINES,1,2)
      WRITE(6,232)  (X(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,233)
      CALL LINECT(LINES,2,2)
      WRITE(6,234)  (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,2,2)
      A=12.0
      DO 30 J=1,N
30 C1(J)=C1(J)/(A*DX**2)
      WRITE(6,234)  (C1(J),J=1,N)
      CALL LINECT(LINES,4,2)

```



```

WRITE(6,223)
WRITE(6,240)
DO 36 J=1,N
DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(A*DX**2)

```

```

36 CONTINUE

```

```

C FIND OUT THE EIGENVALUES AND EIGENVECTORS OF
C THE COEFFICIENT MATRIX USING S.S.P
CALL CS006A(MATRIX,B,VECTOR,E,XX,X1,N,K,3,
1&270,&271)

```

```

C THE DESCRIPTION OF PARAMETERS

```

```

C MATRIX= THE ORIGINAL COEFFICIENT MATRIX (N,N)

```

```

C B= THE MARIX USED IN CALCULATIONS

```

```

C VECTOR= THE EIGENVECTOR MATRIX(N,N), STORED

```

```

C COLUMNWISE

```

```

C E= THE EIGENVALUES IN DESCENDING ORDER

```

```

C (VECTOR OF LENGTH N)

```

```

C XX,X1= THE VECTORS OF LENGTH N, USED IN

```

```

C CALCULATIONS

```

```

C N= THE DIMENSIONS OF MATRIX

```

```

C K= THE NUMBER OF EIGENVALUES FOUND (K=N,

```

```

C UNLESS TOO MANY ITERATIONS

```

```

C M=3

```

```

C N1=270 (THE STATEMENT NO. TO WHICH THE CONTROL
C IS TRANSFERRED IF N.LE.2)

```

```

C N2= THE STATEMENT NO. TO WHICH THE CONTROL IS
C IS PASSED IF TOO MANY ITERATIONS ARE REQUIRED

```

```

C TO FIND THE K'TH EIGENVALUE

```

```

DO 31 J=1,N

```

```

CALL LINECT(LINES,1,2)

```

```

31 WRITE(6,241)(MATRIX(J,K),K=1,N)

```

```

WRITE(6,220)

```

```

LINES=9

```

```

CALL LINECT(LINES,3,2)

```

```

WRITE(6,223)

```

```

WRITE(6,256)

```

```

CALL LINECT(LINES,2,2)

```

```

WRITE(6,232) (E(J),J=1,N)

```

```

CALL LINECT(LINES,3,2)

```

```

WRITE(6,223)

```

```

WRITE(6,257)

```

```

DO 39 K=1,N

```

```

CALL LINECT(LINES,3,2)

```

```

WRITE(6,232) (VECTOR(K,J),J=1,N)

```

```

39 WRITE(6,223)

```

```

DO 53 I=1,N

```

```

DO 53 J=1,N

```

```

VICTDR(I,J)=VECTOR(I,J)

```

```

53 CONTINUE

```

```

C CALCULATE THE INVERSE OF THE MATRIX OF EIGENVECTORS

```



```

CALL MINV(VICTOR,N,D,XX,X1)
CALL CHECK(VECTOR,E,VICTOR,N,W)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,1,2)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,4,2)
WRITE(6,232) (W(J,K),K=1,N)
33 WRITE(6,223)
CALL SEMIAN(N,VAR,VECTOR,C1,C1, E ,TIME,NT,
1CEVR,VICTOR)
WRITE(6,223)
WRITE(6,225)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,248)
DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
STOP
270 WRITE(6,272)
STOP
271 WRITE(6,273)
STOP

```

C

FORMAT STATEMENTS

```

1  FORMAT(1X,2I4)
2  FORMAT(1X,F13.8, 4F14.8)
3  FORMAT(11F7.3)
4  FORMAT(1X,F16.8)
5  FORMAT(10F8.5)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
111HDIMENSIONAL/25X,22H  HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
18HEQUATION/20X,19HUSING ORDINARY B.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,27HORIGIAL COEFFICIENT MATRIX)
241 FORMAT(1H,10X, 5F8.2)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,

```



```
12H 3, 8X, 2H 4, 8X, 2H 5)
251 FCRMAT(1H, 15X, F6.1, 2X, 5F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
127HORIGIAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
127HORIGIAL COEFFICIENT MATRIX)
272 FORMAT(1H,10X,6HN.LE.2)
273 FORMAT(1H,10X,19HTOO MANY ITERATIONS)
END
```


CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.131200 0.353500 0.545400 0.727200 0.909000

INITIAL CONDITION VECTOR

0.0 0.0 0.0 0.0 0.0

BOUNDARY CONDITION VECTOR

3.8015 -0.9626 0.0 0.0 0.0

ORIGINAL COEFFICIENT MATRIX

12.10	-3.30	0.0	0.0	0.0
-11.74	15.13	-4.40	0.05	0.0
0.96	-11.74	15.13	-4.40	0.05
0.0	0.96	-11.74	15.13	-4.46
0.0	0.0	0.96	-11.69	10.73

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

27.077545	20.050812	12.397358	5.281773	2.405521
-----------	-----------	-----------	----------	----------

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.050344	-0.075309	0.136606	-0.117593	0.057409
-----------	-----------	----------	-----------	----------

0.228294	0.225607	-0.012210	-0.217752	0.103630
----------	----------	-----------	-----------	----------

-0.475846	-0.000343	-0.373484	-0.099710	0.340155
-----------	-----------	-----------	-----------	----------

0.674763	-0.605051	-0.150867	0.336174	0.553902
----------	-----------	-----------	----------	----------

-0.510591	0.757632	0.003407	0.905661	0.758753
-----------	----------	----------	----------	----------

CHECK OF SIMILARITY TRANSFORMATION

12.102222	-3.320033	-0.000034	-0.000042	-0.000007
-11.735241	15.127013	-4.401171	0.045853	0.000012
0.962638	-11.735296	15.128030	-4.401245	0.045886
0.000021	0.002613	-11.735307	15.128030	-4.355353
0.000031	-0.003021	0.962647	-11.689433	13.726751

SOLUTION OF THE DISPERSION MODELEQUATION USING ORDINARY B.C. SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.525958	0.176475	0.033404	0.001545	-0.000943
0.2	0.729804	0.414208	0.182635	0.058351	0.013554
0.3	0.828855	0.589391	0.349987	0.171427	0.075412
0.4	0.884112	0.703102	0.432555	0.322325	0.177956
0.5	0.917963	0.781717	0.505214	0.427423	0.297956
0.6	0.941100	0.835163	0.592501	0.537235	0.416783
0.7	0.955242	0.874453	0.759974	0.629527	0.524346
0.8	0.968106	0.903401	0.812274	0.705215	0.616776
0.9	0.974021	0.925200	0.852953	0.766372	0.693723
1.0	0.979943	0.941862	0.884690	0.815331	0.756546

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.131800 0.363500 0.545400 0.727200 0.909000

INITIAL CONDITION VECTOR

0.0 0.0 0.0 0.0 0.0

BOUNDARY CONDITION VECTOR

4.1910 -1.4584 0.0 0.0 0.0

ORIGINAL COEFFICIENT MATRIX

7.43	-1.30	0.0	0.0	0.0
-11.23	15.13	-4.40	0.05	0.0
0.96	-11.74	15.13	-4.40	0.05
0.0	0.96	-11.74	15.13	-4.36
0.0	0.0	0.96	-11.69	10.73

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

26.904907 10.321091 10.864983 4.577445 1.085138

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.036304 -0.255386 0.102772 -0.131601 0.145493

0.213509 0.236811 -0.105026 -0.112375 0.251122

-0.471610 -0.262042 -0.364409 0.074255 0.390473

0.679294 -0.570435 -0.040871 0.456189 0.549047

-0.513833 0.770399 0.913605 0.869700 0.673379

CHECK OF SIMILARITY TRANSFORMATION

7.491765 -3.487044 0.000008 -0.000007 -0.000012

-11.230912 15.127830 -4.401134 0.045861 0.007001

0.962643 -11.735320 15.123722 -4.401243 0.045830

0.000032 0.962646 -11.735299 15.123739 -4.355360

-0.000033 -0.000010 0.962637 -11.684443 10.725783

SOLUTION OF THE DISPERSION MODELEQUATION USING DAMCKWERTS B.C. SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.373901	0.095462	0.017080	0.000637	-0.000509
0.2	0.431934	0.255337	0.105237	0.032302	0.007051
0.3	0.602171	0.396574	0.221157	0.102780	0.043173
0.4	0.685539	0.509758	0.335712	0.195124	0.109570
0.5	0.750113	0.600102	0.438692	0.293664	0.195402
0.6	0.790730	0.672439	0.528449	0.383277	0.288934
0.7	0.835604	0.730726	0.604878	0.477332	0.381666
0.8	0.865565	0.777995	0.669534	0.556039	0.466534
0.9	0.897535	0.815546	0.723957	0.624845	0.547023
1.0	0.900895	0.843135	0.769822	0.684204	0.616295


```

C      SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C      DIMENSIONAL HOMOGENEOUS CASE
C      USING HIGHER ORDER CORRECT MONOTONE TYPE
C      APPROXIMATIONS
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
C      REAL MATRIX(10,10),B(10,10),VECTOR(10,10),E(10),
C      1XX(10),X1(10),W(10,10),X(10),VAR(10),CI(10),
C      2C1(10),CEVR(15,10),TIME(15),D,VICTOR(10,10),
C      3X2(10),X3(10),A
C      READ THE DATA
C      READ( 5,1)  N,NT
C      READ(5,5)  ((MATRIX(I,J),J=1,N),I=1,N)
C      READ( 5,2 )  (X(J),J=1,N)
C      READ( 5,2 )  (CI(J),J=1,N)
C      READ(5,2)  (C1(J),J=1,N)
C      READ(5,3)  (TIME(J), J=1,NT)
C      READ(5,4) DX
C      WRITE(6,223)
C      LINES=9
C      CALL LINECT(LINES,4,2)
C      WRITE(6,253) DX
C      WRITE(6,220)
C      LINES =9
C      CALL LINECT(LINES,4,2)
C      WRITE(6,224)
C      WRITE(6,223)
C      WRITE(6,231)
C      CALL LINECT(LINES,1,2)
C      WRITE(6,232) (X(J),J=1,N)
C      CALL LINECT(LINES,4,2)
C      WRITE(6,223)
C      WRITE(6,223)
C      CALL LINECT(LINES,2,2)
C      WRITE(6,234) (CI(J),J=1,N)
C      CALL LINECT(LINES,4,2)
C      WRITE(6,223)
C      WRITE(6,235)
C      CALL LINECT(LINES,2,2)
C      A=12.0
C      DO 30 J=1,N
30  C1(J)=C1(J)/(A*DX**2)
C      WRITE(6,234) (C1(J),J=1,N)

```



```

CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,240)
DO 36 J=1,N
DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(A*DX**2)
36 CONTINUE
C   FIND OUT THE EIGENVALUES AND EIGENVECTORS OF
C   THE COEFFICIENT MATRIX USING S.S.P
CALL CS006A(MATRIX,B,VECTOR,E,XX,X1,N,K,3,
1&270,&271)
C   THE DESCRIPTION OF PARAMETERS
C   MATRIX= THE ORIGINAL COEFFICIENT MATRIX (N,N)
C   B= THE MARIX USED IN CALCULATIONS
C   VECTOR= THE EIGENVECTOR MATRIX(N,N), STORED
C   COLUMNWISE
C   E= THE EIGENVALUES IN DESCENDING ORDER
C   (VECTOR OF LENGTH N)
C   XX,X1= THE VECTORS OF LENGTH N, USED IN
C   CALCULATIONS
C   N= THE DIMENSIONS OF MATRIX
C   K= THE NUMBER OF EIGENVALUES FOUND (K=N,
C   UNLESS TOO MANY ITERATIONS
C   M=3
C   N1=270 (THE STATEMENT NO. TO WHICH THE CONTROL
C   IS TRANSFERRED IF N.LE.2)
C   N2= THE STATEMENT NO. TO WHICH THE CONTROL IS
C   IS PASSED IF TOO MANY ITERATIONS ARE REQUIRED
C   TO FIND THE K'ITH EIGENVALUE
DO 31 J=1,N
CALL LINECT(LINES,1,2)
31 WRITE(6,241)(MATRIX(J,K),K=1,N)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,256)
CALL LINECT(LINES,2,2)
WRITE(6,232) (E(J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,257)
DO 39 K=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
DO 53 I=1,N
DO 53 J=1,N
VECTOR(I,J)=VECTOR(I,J)
53 CONTINUE

```



```
240 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX)
241 FORMAT(1H,10X,10F6.1)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID PUINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
      12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
      18X,2H 9, 8X, 2H10)
251 FORMAT(1H, 15X, F5.1, 2X, 5F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
      127HORIGINAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
      127HORIGINAL COEFFICIENT MATRIX)
272 FORMAT(1H,10X,6HN.LE.2)
273 FORMAT(1H,10X,19HTOO MANY ITERATIONS)
      END
```


CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

27.2990	-2.7124	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

ORIGINAL COEFFICIENT MATRIX

44.1	-16.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-36.4	55.1	-22.4	1.0	0.0	0.0	0.0	0.0	0.0	0.0
2.7	-36.4	55.1	-22.4	1.0	0.0	0.0	0.0	0.0	0.0
0.0	2.7	-36.4	55.1	-22.4	1.0	0.0	0.0	0.0	0.0
0.0	0.0	2.7	-36.4	55.1	-22.4	1.0	0.0	0.0	0.0
0.0	0.0	0.0	2.7	-36.4	55.1	-22.4	1.0	0.0	0.0
0.0	0.0	0.0	0.0	2.7	-36.4	55.1	-22.4	1.0	0.0
0.0	0.0	0.0	0.0	0.0	2.7	-36.4	55.1	-22.4	1.0
0.0	0.0	0.0	0.0	0.0	0.0	2.7	-36.4	55.1	-21.4
0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.7	-35.4	32.7

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

112.101074	102.556976	88.418991	71.842300	54.941483
39.200470	25.443909	14.351689	6.569824	2.377954

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

0.016973	-0.030242	0.047206	-0.067170	-0.085875
0.093932	-0.085530	0.065185	-0.040252	0.018745

-0.068706	0.105235	-0.124539	0.110934	0.055429
0.027383	-0.094972	0.115421	-0.089918	0.046552

0.137568	-0.166195	0.109870	0.017926	0.135291
-0.138490	0.020865	0.104256	-0.136328	0.084928

-0.222538	0.173399	0.034768	-0.195730	-0.108149
-0.124987	0.179728	0.003109	-0.160162	0.135026

0.316610	-0.088619	-0.232363	0.138914	-0.205179
0.151956	0.190363	-0.162632	-0.138719	0.197106

-0.406660	-0.099124	0.298734	0.199378	0.203525
0.290904	-0.053376	-0.300517	-0.052341	0.269944

0.472021	0.350453	-0.078042	-0.397378	0.305848
-0.077450	-0.374510	-0.283529	0.106383	0.350091

-0.483906	-0.565686	-0.367767	0.016633	-0.372136
-0.516660	-0.380644	-0.030099	0.322362	0.430994

0.406005	0.602128	0.689754	0.632619	-0.446527
-0.174397	0.131264	0.402997	0.549914	0.502017

-0.197789	-0.327520	-0.456777	-0.571934	0.666797
0.737943	0.780681	0.781722	0.711643	0.547702

CHECK OF SIMILARITY TRANSFORMATION

44.097900	-16.799454	0.000079	-0.000031	0.000022
0.000022	-0.000020	-0.000004	0.000018	-0.000003
-36.398300	55.122498	-22.408096	0.962735	-0.000028
0.000058	-0.000075	0.000023	-0.000018	-0.000006
2.712015	-36.398483	55.122742	-22.408295	0.962809
0.000009	0.000035	0.000019	0.000011	0.000006
0.000045	2.712020	-36.398453	55.122726	-22.408295
0.962786	-0.000016	0.000000	0.000010	0.000009
-0.000120	0.000216	2.711850	-36.398239	55.122528
-22.408112	0.962710	0.000063	-0.000052	0.000005
-0.000008	0.000045	0.000042	2.712017	-36.398392
55.122711	-22.408264	0.962815	-0.000009	-0.000005
0.000011	0.000013	0.000049	0.000032	2.711937
-36.398422	55.122726	-22.408264	0.962829	0.000001
0.000029	0.000013	-0.000103	-0.000040	0.000055
2.712003	-36.398407	55.122772	-22.408279	0.962803
0.000117	-0.000097	0.000017	-0.000011	-0.000029
0.000042	2.711966	-36.398453	55.122726	-21.436279
-0.000203	0.000009	0.000012	0.000035	-0.000011
0.000026	0.000071	2.711989	-35.436539	32.724518

SOLUTION OF THE DISPERSION MODELEQUATION
USING ORDINARY B.C.
SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS					
TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.768596	0.511058	0.288764	0.137029	0.053947
0.2	0.881985	0.728629	0.558586	0.394602	0.255489
0.3	0.926991	0.826915	0.705505	0.572762	0.440634
0.4	0.950738	0.881351	0.793119	0.690146	0.578828
0.5	0.965072	0.915059	0.849574	0.770042	0.679711
0.6	0.974442	0.937449	0.888040	0.826434	0.754214
0.7	0.980905	0.953067	0.915353	0.867470	0.810149
0.8	0.985539	0.964359	0.935353	0.898048	0.852749
0.9	0.988958	0.972738	0.950332	0.921236	0.885547
1.0	0.991533	0.979076	0.961735	0.939041	0.910994

CONCENTRATIONS AT GRID POINTS					
TIME	6	7	8	9	10
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.017281	0.004329	0.000762	0.000053	-0.000026
0.2	0.150957	0.081094	0.039497	0.017585	0.008199
0.3	0.320183	0.219328	0.141959	0.088804	0.060177
0.4	0.466820	0.361881	0.271105	0.201137	0.160016
0.5	0.583434	0.487360	0.398774	0.326481	0.282249
0.6	0.674449	0.591811	0.512800	0.446281	0.404728
0.7	0.745379	0.676704	0.609602	0.552073	0.515714
0.8	0.800790	0.744875	0.689491	0.641463	0.610899
0.9	0.844190	0.799244	0.754322	0.715068	0.689981
1.0	0.878254	0.842425	0.806393	0.774725	0.754431

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

BOUNDARY CONDITION VECTOR

8.8062	-0.8750	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0

ORIGINAL COEFFICIENT MATRIX

25.6	-16.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-34.6	55.1	-22.4	1.0	0.0	0.0	0.0	0.0	0.0	0.0
2.7	-36.4	55.1	-22.4	1.0	0.0	0.0	0.0	0.0	0.0
0.0	2.7	-36.4	55.1	-22.4	1.0	0.0	0.0	0.0	0.0
0.0	0.0	2.7	-36.4	55.1	-22.4	1.0	0.0	0.0	0.0
0.0	0.0	0.0	2.7	-36.4	55.1	-22.4	1.0	0.0	0.0
0.0	0.0	0.0	0.0	2.7	-36.4	55.1	-22.4	1.0	0.0
0.0	0.0	0.0	0.0	0.0	2.7	-36.4	55.1	-22.4	1.0
0.0	0.0	0.0	0.0	0.0	0.0	2.7	-36.4	55.1	-21.4
0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.7	-35.4	32.7

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

112.009277	102.172089	87.492706	70.087936	52.168976
35.612411	21.742416	11.351755	4.804333	1.870262

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

0.012303	-0.021567	0.032781	-0.045738	-0.059906
0.073653	-0.084104	0.087779	-0.081985	0.073412
-0.063276	0.098295	-0.120761	0.121106	0.094726
-0.043874	-0.019339	0.074477	-0.101513	0.103720
0.132289	-0.165367	0.124363	-0.018187	0.098225
-0.153705	0.108966	0.005389	-0.105016	0.141270
-0.218086	0.180545	0.011053	-0.182667	-0.154940
-0.044376	0.187538	-0.109499	-0.081791	0.186393
0.313667	-0.102186	-0.219294	0.173123	-0.157611
0.215768	0.092712	-0.225165	-0.021907	0.238814
-0.405712	-0.084109	0.309394	0.161338	0.253650
0.233862	-0.170255	-0.268513	0.080551	0.297301
0.473150	0.340202	-0.104371	-0.408558	0.252857
-0.174131	-0.393957	-0.167636	0.223412	0.359213
-0.486603	-0.563961	-0.348655	0.058339	-0.415179
-0.509675	-0.289554	0.101712	0.392071	0.419933
0.409079	0.607074	0.690683	0.619149	-0.405490
-0.100298	0.221802	0.471511	0.555941	0.472171
-0.199485	-0.331792	-0.464158	-0.582987	0.681081
0.752103	0.787203	0.768870	0.667521	0.505383

CHECK OF SIMILARITY TRANSFORMATION

25.605331	-16.799500	0.000062	-0.000007	-0.000024
-0.000004	0.000009	-0.000003	-0.000003	-0.000001

-34.560837	55.122498	-22.408051	0.962788	-0.000034
0.000035	-0.000016	0.000030	-0.000021	0.000016

2.711977	-36.398499	55.122696	-22.408249	0.962797
-0.000012	-0.000005	-0.000017	-0.000007	-0.000001

0.000025	2.712042	-36.398437	55.122726	-22.408279
0.962813	0.000017	0.000002	0.000004	-0.000005

-0.000005	0.000113	2.711880	-36.398300	55.122604
-22.408173	0.962729	0.000050	-0.000019	0.000009

-0.000060	-0.000013	-0.000059	2.712010	-36.398499
55.122726	-22.408310	0.962812	-0.000014	0.000004

0.000059	0.000037	0.000068	0.000042	2.712080
-36.398468	55.122787	-22.408264	0.962823	-0.000002

0.000106	-0.000098	0.000141	-0.000093	-0.000016
2.712029	-36.398468	55.122772	-22.408279	0.962811

-0.000175	0.000113	-0.000150	0.000145	-0.000015
0.000017	2.712030	-36.398483	55.122757	-21.436295

0.000074	-0.000082	-0.000007	-0.000156	0.000019
0.000081	-0.000006	2.712049	-35.436569	32.724548

SOLUTION OF THE DISPERSION MODELEQUATION
 USING DANCKWERTS B.C.
 SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS					
TIME	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.421237	0.256385	0.134540	0.060021	0.022419
0.2	0.593183	0.456578	0.327679	0.217918	0.133593
0.3	0.697079	0.588243	0.475241	0.366089	0.267957
0.4	0.767475	0.680663	0.585624	0.487329	0.391228
0.5	0.818023	0.748356	0.669428	0.584181	0.496380
0.6	0.855651	0.799406	0.734131	0.661500	0.584035
0.7	0.884371	0.838736	0.784829	0.723551	0.656582
0.8	0.906706	0.869540	0.825046	0.773665	0.716520
0.9	0.924329	0.893980	0.857270	0.814373	0.766045
1.0	0.938394	0.913569	0.883298	0.847599	0.806992

CONCENTRATIONS AT GRID POINTS					
TIME	6	7	8	9	10
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.006853	0.001639	0.000273	0.000017	-0.000008
0.2	0.075152	0.038629	0.018078	0.007755	0.003489
0.3	0.185817	0.121844	0.075685	0.045508	0.029805
0.4	0.302418	0.225014	0.161976	0.115625	0.089211
0.5	0.410224	0.330029	0.260177	0.205582	0.173079
0.6	0.504997	0.428332	0.358808	0.302536	0.268226
0.7	0.586419	0.516498	0.451448	0.397654	0.364387
0.8	0.655533	0.593627	0.535051	0.485924	0.455271
0.9	0.713782	0.660042	0.608597	0.565027	0.537685
1.0	0.762649	0.716629	0.672201	0.634309	0.610435


```

C          PROGRAM FOR INTERPOLATION
C  INTERPOLATE THE VALUES OF CONCENTRATION
C  CORRESPONDING TO ONE GRID FROM THOSE
C  OF A HIGHER POINT GRID
C  N= THE NUMBER OF GRID POINTS ( THE VALUES
C  TO BE INTERPOLATED)
C  NN= THE NUMBER OF GRID POINTS ( GREATER THAN
C  ABOVE)
C  NT= THE TOTAL NUMBER OF TIMES
C  GRIDX=THE DIMENSIONLESS DISTANCES OF GRID POINTS
C  (CORRESPONDING TO THE VALUES TO BE INTERPOLATED)
C  GRIDN=THE DIMENSIONLESS DISTANCES OF GRID POINTS
C  (CORRESPONDING TO THE HIGHER POINT GRID)
C  REAL GRIDX(5),GRIDN(10),TIME(15),CONC(15,5),
1CEVR(15,5),WORK(150)
C  REAL CINTP(15,5),ERROR(15,5),X,F(150),ARG(10),
1Z(10),Y,YY(10),VAL(150)
C  INTEGER I,J,N,NN,NT
C  READ(5,1)  N,NN,NT
C  READ(5,2)  (TIME(J),J=1,NT)
C  DO 3 J=1,NT
C  READ(5,6)  (CEVR(J,K),K=1,NN)
3  CONTINUE
C  DO 5 J=1,NT
C  READ(5,6)  (CONC(J,K),K=1,N)
5  CONTINUE
C  READ(5,12) (GRIDX(J),J=1,N)
C  READ(5,13) (GRIDN(J),J=1,NN)
C  WRITE(6,220)
C  LINES=10
C  CALL LINECT(LINES,4,2)
C  WRITE(6,264)
C  CALL LINECT(LINES,3,2)
C  WRITE(6,265) (GRIDX(I),I=1,N)
C  WRITE(6,222)
C  WRITE(6,266)
C  CALL LINECT(LINES,3,2)
C  WRITE(6,265) (GRIDN(I),I=1,NN)
C  WRITE(6,223)
C  WRITE(6,225)
C  LINES=9
C  CALL LINECT(LINES,4,2)
C  WRITE(6,245)
C  WRITE(6,223)
C  WRITE(6,246)
C  WRITE(6,247)
C  WRITE(6,248)
C  DO 7 J=1,NT
7  WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
C  WRITE(6,223)

```



```

WRITE(6,246)
WRITE(6,249)
DO 8 J=1,NT
8 WRITE(6,251)  TIME(J), (CEVR(J,K),K=6,10)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,3,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,250)
WRITE(6,248)
DO 9 J=1,NT
9 WRITE(6,251)  TIME(J), (CONC(J,K),K=1,5)
DO 14 JJ=1,NN
Z(JJ)=GRIDN(JJ)
14 CONTINUE

C
C   THE TABLE OF Z VS F READY FOR ONE VALUE OF TIME
C
C
C   ORDER THE TABLE USING  S.S.P
C

IROW=10
ICOL=1
NDIM=10
DO 19 J=1,NT
DO 19 I=1,N
X=GRIDX(I)
DO 31 JJ=1,NN
F(JJ)=CEVR(J,JJ)
31 CONTINUE
CALL ATSG(X,Z,F,WORK,IROW,ICOL,ARG,VAL,NDIM)
EPS=0.00001
CALL ALI(X,ARG,VAL,Y,NDIM,EPS,IER)
YY(I)=Y
CINTP(J,I)=YY(I)
19 CONTINUE
WRITE(6,223)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,260)
WRITE(6,248)
DO 20 J=1,NT
20 WRITE(6,251)  TIME(J), (CINTP(J,K),K=1,5)
DO 27 J=1,NT
DO 27 K=1,N
27 ERROR(J,K)=CINTP(J,K)-CONC(J,K)
WRITE(6,223)
WRITE(6,255)

```



```
WRITE(6,223)
```

```
WRITE(6,248)
```

```
DO 28 J=1,NT
```

```
28 WRITE(6,251) TIME(J), (ERROR(J,K),K=1,5)
```

C

FORMAT STATEMENTS

```
1 FORMAT(1X,3I3)
```

```
2 FORMAT(10F7.3)
```

```
6 FORMAT(5F16.6)
```

```
12 FORMAT(1X,F13.8,4F14.8)
```

```
13 FORMAT(10F8.5)
```

```
220 FORMAT(1H2)
```

```
222 FORMAT(1H,//)
```

```
223 FORMAT(1H,/)
```

```
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,  
18HEQUATION/20X,19HUSING ORDINARY B.C.)
```

```
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
```

```
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
```

```
247 FORMAT(1H,40X,14HTEN POINT GRID)
```

```
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,  
12H 3, 8X, 2H 4, 8X, 2H 5)
```

```
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,  
18X,2H 9, 8X, 2H10)
```

```
250 FORMAT(1H,40X,15HFIVE POINT GRID)
```

```
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
```

```
260 FORMAT(1H,30X,20H INTERPOLATED VALUES)
```

```
255 FORMAT(1H,30X,18H ASSOCIATED ERRORS)
```

```
264 FORMAT(1H,25X,28HGRID POINTS(FIVE POINT GRID))
```

```
265 FORMAT(1H,10X,5F10.6)
```

```
266 FORMAT(1H,25X,27HGRID POINTS(TEN POINT GRID))
```

```
STOP
```

```
END
```


GRID POINTS(FIVE POINT GRID)
0.181800 0.363600 0.545400 0.727200 0.909000

GRID POINTS(TEN POINT GRID)
0.095240 0.190480 0.285720 0.380960 0.476200
0.571440 0.666680 0.761920 0.857160 0.952400

SOLUTION OF THE DISPERSION MODELEQUATION
USING ORDINARY B.C.
SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS TEN POINT GRID					
TIME	1	2	3	4	5
0.1	0.768596	0.511058	0.288764	0.137029	0.053947
0.2	0.881985	0.728629	0.558586	0.394602	0.255489
0.3	0.926991	0.826915	0.705505	0.572762	0.440634
0.4	0.950738	0.881351	0.793119	0.690146	0.578828
0.5	0.965072	0.915059	0.849574	0.770042	0.679711
0.6	0.974442	0.937449	0.888040	0.826434	0.754214
0.7	0.980905	0.953067	0.915353	0.867470	0.810149
0.8	0.985539	0.964359	0.935353	0.898048	0.852749
0.9	0.988958	0.972738	0.950332	0.921236	0.885547
1.0	0.991533	0.979076	0.961735	0.939041	0.910994

CONCENTRATIONS AT GRID POINTS					
TIME	6	7	8	9	10
0.1	0.525958	0.176475	0.033404	0.001545	-0.000949
0.2	0.729894	0.419208	0.182635	0.058351	0.013554
0.3	0.828855	0.589391	0.349980	0.171427	0.075412
0.4	0.884112	0.703162	0.492555	0.302325	0.177966
0.5	0.917963	0.780717	0.605214	0.427423	0.297956
0.6	0.940100	0.835163	0.692501	0.537235	0.416783
0.7	0.955292	0.874453	0.759974	0.629527	0.524346
0.8	0.966106	0.903461	0.812274	0.705215	0.616776
0.9	0.974021	0.925260	0.852953	0.766372	0.693729
1.0	0.979933	0.941862	0.884690	0.815331	0.756546

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS FIVE-POINT GRID

TIME	1	2	3	4	5
0.1	0.525958	0.176475	0.033404	0.001545	-0.000949
0.2	0.729894	0.419208	0.182635	0.058351	0.013554
0.3	0.828855	0.589391	0.349980	0.171427	0.075412
0.4	0.884112	0.703162	0.492555	0.302325	0.177966
0.5	0.917963	0.780717	0.605214	0.427423	0.297956
0.6	0.940100	0.835163	0.692501	0.537235	0.416783
0.7	0.955292	0.874453	0.759974	0.629527	0.524346
0.8	0.966106	0.903461	0.812274	0.705215	0.616776
0.9	0.974021	0.925260	0.852953	0.766372	0.693729
1.0	0.979933	0.941862	0.884690	0.815331	0.756546

INTERPOLATED VALUES

TIME	1	2	3	4	5
0.1	0.533895	0.159514	0.435134	0.067952	0.001229
0.2	0.743669	0.423191	0.629377	0.256354	0.026204
0.3	0.837052	0.597262	0.743143	0.432569	0.107545
0.4	0.888495	0.709725	0.815145	0.569510	0.223746
0.5	0.920265	0.785438	0.863360	0.671668	0.347134
0.6	0.941337	0.838500	0.897094	0.747771	0.463418
0.7	0.956007	0.876922	0.921501	0.804995	0.565555
0.8	0.966605	0.905451	0.939609	0.848491	0.651676
0.9	0.974464	0.927033	0.953287	0.881862	0.722530
1.0	0.980405	0.943576	0.963757	0.907648	0.779925

ASSOCIATED ERRORS

TIME	1	2	3	4	5
0.1	0.007937	-0.016961	0.401730	0.066406	0.002178
0.2	0.013775	0.003983	0.446742	0.198003	0.012650
0.3	0.008197	0.007871	0.393163	0.261142	0.032133
0.4	0.004383	0.006563	0.322590	0.267185	0.045780
0.5	0.002302	0.004721	0.258146	0.244245	0.049178
0.6	0.001237	0.003337	0.204593	0.210536	0.046635
0.7	0.000715	0.002469	0.161527	0.175468	0.041209
0.8	0.000499	0.001990	0.127335	0.143276	0.034900
0.9	0.000443	0.001773	0.100334	0.115490	0.028801
1.0	0.000472	0.001714	0.079067	0.092317	0.023379


```

C          PROGRAM FOR INTERPOLATION
C  INTERPOLATE THE VALUES OF CONCENTRATION
C  CORRESPONDING TO ONE GRID FROM THOSE
C  OF A HIGHER POINT GRID
C  N= THE NUMBER OF GRID POINTS ( THE VALUES
C  TO BE INTERPOLATED)
C  NN= THE NUMBER OF GRID POINTS ( GREATER THAN
C  ABOVE)
C  NT= THE TOTAL NUMBER OF TIMES
C  X= THE DIMENSIONLESS DISTANCES OF THE GRID
C  POINTS CORRESPONDING TO THE VALUES TO BE
C  INTERPOLATED)
C  XX= THE DIMENSIONLESS DISTANCES OF THE GRID
C  POINTS (CORRESPONDING TO THE HIGHER POINT GRID)
REAL    X(5),XX(15),TIME(15),CONC(15,5),
1CEVR(15,5),CGRID(15,5)
REAL CINTP(15,5),EPROR(15,5)
INTEGER I,J,N,NN,NT
READ(5,1)  N,NN,NT
READ(5,2)  (TIME(J),J=1,NT)
DO 3 J=1,NT
  READ(5,6)  (CEVR(J,K),K=1,NN)
3 CONTINUE
DO 5 J=1,NT
  READ(5,6)  (CONC(J,K),K=1,N)
5 CONTINUE
READ(5,12)  (X(J),J=1,N)
READ(5,13)  (XX(J),J=1,NN)
WRITE(6,222)
LINES=10
CALL LINECT(LINES,4,2)
WRITE(6,261)
CALL LINECT(LINES,3,2)
WRITE(6,262) (X(I),I=1,N)
WRITE(6,222)
WRITE(6,263)
CALL LINECT(LINES,3,2)
WRITE(6,262) (XX(I),I=1,NN)
WRITE(6,223)
WRITE(6,225)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,247)
WRITE(6,248)
DO 7 J=1,NT
7 WRITE(6,251)  TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)

```



```

WRITE(6,246)
WRITE(6,249)
DO 8 J=1,NT
8 WRITE(6,251)  TIME(J), (CEVR(J,K),K=6,10)
WRITE(6,220)
LINES=10
CALL LINECT(LINES,3,2)
WRITE(6,245)
WRITE(6,223)
WRITE(6,246)
WRITE(6,250)
WRITE(6,248)
DO 9 J=1,NT
9 WRITE(6,251)  TIME(J), (CONC(J,K),K=1,5)
CALL CALCU(10,N,NT,CEVR,1,X,TIME, CINTP,XX)
WRITE(6,223)
LINES=9
CALL LINECT(LINES,4,2)
WRITE(6,260)
WRITE(6,248)
DO 10 J=1,NT
10 WRITE(6,251)  TIME(J), (CINTP(J,K),K=1,5)
DO 27 J=1,NT
DO 27 K=1,N
27 ERROR(J,K)=CINTP(J,K)-CONC(J,K)
WRITE(6,223)
WRITE(6,255)
WRITE(6,223)
WRITE(6,248)
DO 11 J=1,NT
11 WRITE(6,251)  TIME(J), (ERROR(J,K),K=1,5)
C      FORMAT STATEMENTS
1 FORMAT(1X,3I3)
2 FORMAT(10F7.3)
6 FORMAT(5F16.6)
12 FORMAT(1X,F13.8,4F14.8)
13 FORMAT(10F8.5)
220 FORMAT(1H2)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
18HEQUATION/20X,21HUSING DANCKWERTS B.C.)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
247 FORMAT(1H,40X,14HTEN POINT GRID)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
18X,2H 9, 8X, 2H10)
250 FORMAT(1H,40X,15HFIVE POINT GRID)

```



```
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
255 FORMAT(1H, 30X, 18H ASSOCIATED ERRORS)
260 FORMAT(1H, 30X, 20H INTERPOLATED VALUES)
261 FORMAT(1H, 25X, 28HGRID POINTS(FIVE POINT GRID))
262 FORMAT(1H, 10X, 5F10.6)
263 FORMAT(1H, 25X, 27HGRID POINTS(TEN POINT GRID))
  STOP
  END
```


GRID POINTS(FIVE POINT GRID)

0.181800	0.363600	0.545400	0.727200	0.909000
----------	----------	----------	----------	----------

GRID POINTS(TEN POINT GRID)

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400

SOLUTION OF THE DISPERSION MODELEQUATION
 USING DANCKWERTS B.C.
 SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS TEN POINT GRID					
TIME	1	2	3	4	5
0.1	0.421237	0.256385	0.134540	0.060021	0.022419
0.2	0.593183	0.456578	0.327679	0.217918	0.133593
0.3	0.697079	0.588243	0.475241	0.366089	0.267957
0.4	0.767475	0.680663	0.585624	0.487329	0.391228
0.5	0.818023	0.748356	0.669428	0.584181	0.496380
0.6	0.855651	0.799406	0.734131	0.661500	0.584035
0.7	0.884371	0.838736	0.784829	0.723551	0.656582
0.8	0.906706	0.869540	0.825046	0.773665	0.716520
0.9	0.924329	0.893980	0.857270	0.814373	0.766045
1.0	0.938394	0.913569	0.883298	0.847599	0.806992

CONCENTRATIONS AT GRID POINTS					
TIME	6	7	8	9	10
0.1	0.303901	0.095462	0.017080	0.000637	-0.000509
0.2	0.481934	0.256337	0.105237	0.032002	0.007051
0.3	0.601171	0.396574	0.221157	0.102730	0.043173
0.4	0.686539	0.509758	0.335712	0.195124	0.109570
0.5	0.750113	0.600102	0.438892	0.293654	0.195402
0.6	0.798720	0.672439	0.528449	0.389227	0.288934
0.7	0.836604	0.730726	0.604878	0.477382	0.381666
0.8	0.866565	0.777995	0.669534	0.556039	0.468534
0.9	0.890535	0.816546	0.723957	0.624845	0.547033
1.0	0.909885	0.848135	0.769622	0.684204	0.616295

SEMI-ANALYTICAL SOLUTION

CONCENTRATIONS AT GRID POINTS
FIVE POINT GRID

TIME	1	2	3	4	5
0.1	0.303901	0.095462	0.017080	0.000637	-0.000509
0.2	0.481934	0.256337	0.105237	0.032002	0.007051
0.3	0.601171	0.396574	0.221157	0.102780	0.043173
0.4	0.685539	0.509758	0.335712	0.195124	0.109570
0.5	0.750113	0.600102	0.438892	0.293654	0.195402
0.6	0.798720	0.672439	0.528449	0.389227	0.288934
0.7	0.836604	0.730726	0.604878	0.477382	0.381666
0.8	0.866565	0.777995	0.669534	0.556039	0.468534
0.9	0.890535	0.816546	0.723957	0.624845	0.547033
1.0	0.909885	0.848135	0.769622	0.684204	0.616295

INTERPOLATED VALUES

TIME	1	2	3	4	5
0.1	0.269628	0.070547	0.241493	0.034891	-0.001884
0.2	0.468708	0.236214	0.401260	0.151479	0.012433
0.3	0.593334	0.385374	0.522623	0.279966	0.063047
0.4	0.683915	0.505242	0.616282	0.396904	0.141731
0.5	0.755088	0.600020	0.689419	0.497243	0.234347
0.6	0.804905	0.675173	0.747196	0.581572	0.329309
0.7	0.843237	0.735193	0.793313	0.651912	0.421341
0.8	0.873230	0.783492	0.830445	0.710439	0.505186
0.9	0.897009	0.822618	0.860557	0.759102	0.579849
1.0	0.916056	0.854486	0.885114	0.799563	0.645069

ASSOCIATED ERRORS

TIME	1	2	3	4	5
0.1	-0.034273	-0.024915	0.224413	0.034254	-0.001375
0.2	-0.013226	-0.020123	0.296023	0.119477	0.005382
0.3	-0.002837	-0.011200	0.301467	0.177186	0.019874
0.4	0.002376	-0.004516	0.280570	0.201780	0.032161
0.5	0.004975	-0.000082	0.250527	0.203589	0.038945
0.6	0.006185	0.002734	0.218747	0.192345	0.040875
0.7	0.006633	0.004467	0.188435	0.174530	0.039675
0.8	0.006665	0.005497	0.160911	0.154400	0.036652
0.9	0.006474	0.006072	0.136600	0.134257	0.032816
1.0	0.006171	0.006351	0.115492	0.115359	0.028774

APPENDIX F

ONE DIMENSIONAL HOMOGENEOUS CASE

(Various Input Signals)

The partial differential equation is

$$\frac{\partial c}{\partial \theta} = \alpha \frac{\partial^2 c}{\partial z^2} - \frac{\partial c}{\partial z}.$$

The boundary conditions are

$$(i) \quad \text{at } z = 0, \quad c = c_{in}(\theta)$$

$$\text{at } z = 1, \quad \frac{\partial c}{\partial z} = 0$$

$$(ii) \quad \text{at } z = 0, \quad c_{in}(\theta) = c_{z \rightarrow 0+} - \alpha \left(\frac{\partial c}{\partial z} \right)_{z \rightarrow 0+}$$

$$\text{at } z = 1, \quad \frac{\partial c}{\partial z} = 0.$$

The above equation has been solved for three different input signals i.e. $c_{in}(\theta)$

$$(a) \quad \text{STEP INPUT:} \quad c_{in}(\theta) = \text{constant}$$

$$(b) \quad \text{SINE WAVE INPUT:} \quad c_{in}(\theta) = 0.75 + 0.25 \sin \omega \theta$$

$$(c) \quad \text{SQUARE WAVE INPUT:} \quad c_{in}(\theta) = 1 \quad 0 < \theta < c$$

$$= -1 \quad 0 < \theta < 2c$$

$$c_{in}(\theta + 2c) = c_{in}(\theta).$$


```

C      SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C      DIMENSIONAL HOMOGENEOUS CASE
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
      REAL*8 DX,W1,BB,BB1
      DOUBLE PRECISION MATRIX(30,30),VECTOR(30,30)
      DOUBLE PRECISION X(30),VAR(30),CI(30),C1(30),
1TOLERC,W(30,30),CEVR(110,30),TIME(110),CONC(110)
      DOUBLE PRECISION D(30,30),VICTOR(30,30)
C      READ THE DATA
      READ( 5,1) N,NT
      READ(5,5) ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 ) (X(J),J=1,N)
      READ( 5,2 ) (CI(J),J=1,N)
      READ( 5,2 ) (C1(J),J=1,N)
      READ(5,2) (TIME(J), J=1,NT)
      READ(5,4) DX
      NORM=2
      TOLERC=0.D00
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,220)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,223)
      WRITE(6,231)
      CALL LINECT(LINES,1,2)
      WRITE(6,232) (X(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,233)
      CALL LINECT(LINES,2,2)
      WRITE(6,234) (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      DO 30 J=1,N
30 C1(J)=C1(J)/(DX**2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,2,2)
      WRITE(6,234) (C1(J),J=1,N)

```



```

CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,240)
DO 36 J=1,N
DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(DX**2)
36 CONTINUE
DO 31 J=1,N
CALL LINECT(LINES,1,2)
31 WRITE(6,241)(MATRIX(J,K),K=1,N)
CALL TRANS(N,DX,D,MATRIX)
LINES=9
WRITE(6,255)
CALL LINECT(LINES,1,2)
WRITE(6,241) (D(J,J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,259)
DO 50 J=1,N
CALL LINECT(LINES,1,2)
50 WRITE(6,241) (MATRIX(J,K),K=1,N)
CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NORM)
WRITE(6,220)
LINES =9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,242)
CALL LINECT(LINES,2,2)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,243)
DO 32 K=1,N
CALL LINECT(LINES,4,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
32 WRITE(6,223)
CALL CHECK(VECTOR,MATRIX,N,W)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,1,2)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,4,2)
WRITE(6,232) (W(J,K),K=1,N)
33 WRITE(6,223)
C CALCULATE THE TRANSPOSE OF THE MATRIX OF
C THE EIGENVECTORS
DO 40 I=1,N
DO 40 J=1,N
VECTOR(I,J)=VECTOR(J,I)

```



```

40 CONTINUE
C   A=(D(-1)*A(*)*D)
C   A(*)=THE ORIGINAL COEFFICIENT MATRIX
C   D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C   OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C   A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C   COEFFICIENT MATRIX A(*)
C   Q=THE MATRIX OF EIGENVECTORS OF A
C   CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C   COEFFICIENT MATRIX
DO 38 I=1,N
DO 38 J=1,N
VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
WRITE(6,220)
LINES=9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,256)
CALL LINECT(LINES,2,2)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,257)
DO 39 K=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
C   (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
C   QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
C   D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
C   CALCULATE THE PRODUCT (QT*D(-1))
DO 41 I=1,N
DO 41 J=1,N
VICTOR(I,J)=VICTOR(I,J)/D(J,J)
41 CONTINUE
CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
1CEVR,VICTOR)
WRITE(6,223)
WRITE(6,225)
WRITE(6,245)
WRITE(6,223)
WRITE(6,264)
WRITE(6,223)
WRITE(6,246)
WRITE(6,248)
DO 34 J=1,NT
34 WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
WRITE(6,223)
WRITE(6,246)

```



```

WRITE(6,249)
DO 35 J=1,NT
35 WRITE(6,252) TIME(J), (CEVR(J,K),K=6,11 )
C      FORMAT STATEMENTS
1  FORMAT(1X,2I4)
2  FORMAT(10F8.5)
4  FORMAT(1X,F16.8)
5  FORMAT(11F7.4)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ...CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
111HDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
18HEQUATION/20X,19HUSING ORDINARY B.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX)
241 FORMAT(1H,10X,11F6.1)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
18X,2H 9, 8X, 2H10,8X,2H11)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
252 FORMAT(1H, 15X, F6.1, 2X, 6F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
255 FORMAT(1H,10X,9HMATRIX(D)/10X,
119H(DIAGONAL ELEMENTS))
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
127HORIGINAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
127HORIGINAL COEFFICIENT MATRIX)
259 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX/
120X,26H(CONVERTED INTO SYMMETRIC))
264 FORMAT(1H,40X,10HSTEP INPUT)
STOP
END

```


SUBROUTINE TRANS(N,DX,D,MATRIX)

THIS SUBROUTINE CONVERTS THE ORIGINAL COEFFICIENT
MATRIX TO THE REAL SYMMETRIC FORM USING
SIMILARITY TRANSFORMATION

INPUT DATA

DX= THE GRID SPACING

N= THE NUMBER OF GRID POINTS

D=THE DIAGONAL MATRIX ,WITH DIAGONAL ENTERIES

HAVING ALTERNATE SIGNS I.E. $D(I,I)=(-1)**(I)(D(I,I))$
USED FOR SIMILARITY TRANSFORMATION

MATRIX= THE ORIGINAL COEFFICIENT MATRIX (DIAGONALLY
DOMINANT & UNSYMMETRIC), DESTROYED DURING
COMPUTATION AND THE RESULTANT MATRIX IS SYMMETRIC
AND DIAGONALLY DOMANANT.

REAL*8 DX,ALPHA,BETA

DOUBLE PRECISION D(30,30),MATRIX(30,30)

ALPHA=0.2

BETA=DX/2.0

D(1,1)=1.0

CALCULATE THE DIAGONAL ELEMENTS OF MATRIX D.

NN=N-3

DO 100 I=1,NN

II=I+1

$D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))$

100 CONTINUE

$D(10,10)=D(9,9)*DSQRT((4./3.)*(ALPHA+BETA)/$
 $1(ALPHA-BETA))$

$D(11,11)=D(10,10)*DSQRT((6.0*ALPHA)/(2.0*$
 $1ALPHA-BETA))$

DO 102 I=1,11,2

$D(I,I)=-D(I,I)$

102 CONTINUE

CALCULATE THE COEFFICIENT MATRIX CONVERTED INTO
THE SYMMETRIC ONE

DO 101 I=1,N

DO 101 J=1,N

$MATRIX(I,J)=(MATRIX(I,J)*D(J,J))/(D(I,I))$

101 CONTINUE

RETURN

END

CONCENTRATION PROFILES-ONE-DIMENSIONAL HOMOGENEOUS MEDIUM

GRID POINTS

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400
1.000000				

INITIAL CCNDITION VECTOR

INITIAL DESCRIPTION VECTOR				
C.C	C.C	O.C	O.O	O.O
O.O	C.O	C.C	O.O	O.O
O.O				

BOUNDARY CONDITION VECTOR

27.2990	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0				

ORIGINAL COEFFICIENT MATRIX

[illegible]

MATRIX (C)

(DIAGONAL ELEMENTS)

-1.0	1.3	-1.6	2.1	-2.6	3.4	-4.3	5.5	-7.0	10.3	-18.9
------	-----	------	-----	------	-----	------	-----	------	------	-------

ORIGINAL COEFFICIENT MATRIX

(CONVERTED INTO SYMMETRIC)

[illegible]

EIGENVALUES

2.369376	84.995322	79.386244	23.383956	6.358656
70.683734	47.501170	13.537093	35.038732	59.728139
238.491119				

EIGENVECTORS

0.089693	0.130317	-0.247625	0.376731	-0.198857
0.341105	-0.430663	-0.299913	0.421505	-0.403418
0.000000				

-0.174751	0.248838	-0.407987	-0.364357	0.350400
0.423407	-0.068425	0.427947	-0.178292	-0.294399
0.000000				

0.250779	0.344837	-0.424575	-0.024343	-0.418570
0.184461	0.419792	-0.310726	-0.346089	0.188577
0.000000				

-0.313848	0.409625	-0.291543	0.387900	0.387147
-0.194439	0.135123	0.015429	0.324684	0.432016
0.000001				

0.360699	0.437337	-0.055772	-0.350815	-0.263609
-0.425814	-0.398323	0.288711	0.208751	0.126692
0.000011				

-0.388911	0.425466	0.199653	-0.048608	0.077350
-0.334116	-0.198410	-0.427391	-0.412983	-0.339561
0.000097				

0.397026	0.375086	0.384721	0.397827	0.127314
0.011083	0.366799	0.321135	-0.034064	-0.374490
0.000871				

-0.384625	0.290756	0.434213	-0.336151	-0.301686
0.347873	0.256688	-0.030837	0.427392	0.066272
0.007809				

0.352348	0.180110	0.330689	-0.072718	0.404276
0.420725	-0.326015	-0.277133	-0.146718	0.422853
0.070001				

-0.261422	0.046040	0.095809	0.352022	-0.355655
0.151004	-0.267157	0.369168	-0.316386	0.209847
0.543464				

0.143580	-0.048146	-0.094398	-0.219894	0.199918
-0.136532	0.198108	-0.216661	0.213928	-0.171918
0.836472				

CHECK OF SIMILARITY TRANSFORMATION

44.098236	21.417811	0.000000	-0.000000	-0.000000
-0.000000	-0.000000	0.000000	0.000000	-0.000000
0.000000				

21.417811	44.098236	21.417811	0.000000	0.000000
-0.000000	0.000000	0.000000	-0.000000	0.000000
-0.000000				

0.000000	21.417811	44.098236	21.417811	0.000000
0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000				

-0.000000	0.000000	21.417811	44.098236	21.417811
0.000000	0.000000	-0.000000	0.000000	0.000000
-0.000000				

-0.000000	0.000000	0.000000	21.417811	44.098236
21.417811	0.000000	-0.000000	-0.000000	0.000000
-0.000000				

-0.000000	-0.000000	0.000000	0.000000	21.417811
44.098236	21.417811	0.000000	-0.000000	0.000000
-0.000000				

-0.000000	0.000000	0.000000	0.000000	0.000000
21.417811	44.098236	21.417811	-0.000000	0.000000
0.000000				

0.000000	0.000000	-0.000000	-0.000000	-0.000000
0.000000	21.417811	44.098236	21.417811	-0.000000
-0.000000				

0.000000	0.000000	-0.000000	0.000000	-0.000000
-0.000000	-0.000000	21.417811	44.098236	24.731155
-0.000000				

-0.000000	-0.000000	-0.000000	0.000000	0.000000
0.000000	0.000000	-0.000000	24.731155	88.196472
95.578286				

0.000000	0.000000	0.000000	-0.000000	-0.000000
-0.000000	0.000000	-0.000000	-0.000000	95.578286
176.392944				

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

2.369376	84.995322	79.386244	23.383956	6.358656
70.683734	47.501170	13.537093	35.038732	59.728139
238.491119				

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.089693	-0.130317	0.247625	-0.376731	0.198857
-0.341105	0.430663	0.299913	-0.421505	0.403418
-0.000000				

-0.222766	0.317209	-0.520086	-0.464468	0.446676
0.539743	-0.087226	0.545530	-0.227280	-0.375289
0.000000				

-0.407520	-0.560366	0.689941	0.039558	0.680182
-0.299753	-0.682168	0.504935	0.562400	-0.306441
-0.000000				

-0.650139	0.848542	-0.603933	0.803538	0.801979
-0.402781	0.279909	0.031961	0.672585	0.894924
0.000003				

-0.952490	-1.154868	0.147275	0.926390	0.696108
1.124438	1.051843	-0.762392	-0.551245	-0.334552
-0.000029				

-1.309165	1.432219	0.672080	-0.163628	0.260377
-1.124712	-0.667895	-1.438698	-1.390199	-1.143042
0.000327				

-1.703696	-1.609548	-1.650892	-1.707134	-0.546325
-0.047558	-1.573987	-1.378036	0.146172	1.606993
-0.003738				

-2.103968	1.590492	2.375226	-1.838808	-1.650278
1.902929	1.404133	-0.168686	2.337914	0.362521
0.042714				

-2.456986	-1.255943	-2.305955	0.507077	-2.819089
-2.933790	2.273365	1.922498	1.023095	-2.948633
-0.488131				

-2.683310	0.472570	0.983412	3.613261	-3.650544
1.549949	-2.742183	3.789255	-3.247485	2.153929

5.578277

-2.719612	0.911959	1.788043	4.165112	-3.786739
2.586121	-3.752454	4.103881	-4.052124	3.256385
-15.844024				

SOLUTION OF THE DISPERSION MODELEQUATION
USING ORDINARY B.C.
SEMI-ANALYTICAL SOLUTION

STEP INPUT

TIME	CONCENTRATIONS AT GRID POINTS				
	1	2	3	4	5
0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.769229	0.510666	0.291627	0.144062	0.062142
0.2	0.881334	0.726742	0.556463	0.393956	0.257437
0.3	0.926401	0.825387	0.703163	0.570310	0.439045
0.4	0.950320	0.880262	0.791248	0.687711	0.576341
0.5	0.964789	0.914294	0.848165	0.768004	0.677251
0.6	0.974250	0.936896	0.886967	0.824772	0.752000
0.7	0.980769	0.952642	0.914494	0.866078	0.808169
0.8	0.985434	0.964001	0.934615	0.896826	0.850944
0.9	0.988868	0.972411	0.949656	0.920111	0.883863
1.0	0.991448	0.978756	0.961082	0.937967	0.909392
1.1	0.993415	0.983610	0.969866	0.951783	0.929299
1.2	0.994932	0.987359	0.976674	0.962539	0.944881
1.3	0.996109	0.990275	0.981980	0.970949	0.957109
1.4	0.997029	0.992552	0.986133	0.977545	0.966723
1.5	0.997748	0.994337	0.989391	0.982728	0.974290
1.6	0.998313	0.995740	0.991953	0.986806	0.980250
1.7	0.998758	0.996843	0.993968	0.990017	0.984948
1.8	0.999108	0.997711	0.995556	0.992548	0.988652
1.9	0.999383	0.998396	0.996808	0.994544	0.991574
2.0	0.999601	0.998935	0.997795	0.996117	0.993878
2.1	0.999772	0.999361	0.998573	0.997358	0.995695
2.2	0.999907	0.999696	0.999186	0.998337	0.997129
2.3	1.000014	0.999961	0.999671	0.999109	0.998261
2.4	1.000098	1.000170	1.000053	0.999719	0.999153
2.5	1.000164	1.000335	1.000354	1.000200	0.999858
2.6	1.000217	1.000465	1.000592	1.000579	1.000413
2.7	1.000258	1.000567	1.000779	1.000878	1.000852
2.8	1.000290	1.000648	1.000927	1.001114	1.001198
2.9	1.000316	1.000712	1.001044	1.001301	1.001471
3.0	1.000336	1.000762	1.001136	1.001448	1.001686
3.1	1.000352	1.000802	1.001209	1.001564	1.001856
3.2	1.000365	1.000833	1.001266	1.001655	1.001990
3.3	1.000375	1.000858	1.001312	1.001727	1.002096
3.4	1.000383	1.000878	1.001347	1.001784	1.002180
3.5	1.000389	1.000893	1.001376	1.001829	1.002245
3.6	1.000394	1.000905	1.001398	1.001865	1.002297
3.7	1.000398	1.000915	1.001415	1.001893	1.002338
3.8	1.000401	1.000922	1.001429	1.001915	1.002371
3.9	1.000403	1.000928	1.001440	1.001932	1.002396
4.0	1.000405	1.000933	1.001449	1.001946	1.002416
4.1	1.000407	1.000937	1.001456	1.001957	1.002432
4.2	1.000408	1.000940	1.001461	1.001966	1.002445
4.3	1.000409	1.000942	1.001465	1.001972	1.002455
4.4	1.000409	1.000944	1.001468	1.001978	1.002463
4.5	1.000410	1.000945	1.001471	1.001982	1.002469
4.6	1.000411	1.000946	1.001473	1.001985	1.002474
4.7	1.000411	1.000947	1.001475	1.001988	1.002477
4.8	1.000411	1.000948	1.001476	1.001990	1.002480

4.9	1.000411	1.000949	1.001477	1.001991	1.002483
5.0	1.000412	1.000949	1.001478	1.001993	1.002485

CONCENTRATIONS AT GRID POINTS						
TIME	6	7	8	9	10	11
0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.1	0.023652	0.008024	0.002450	0.000683	0.000209	0.000148
0.2	0.155311	0.086655	0.044915	0.022105	0.012004	0.010503
0.3	0.320263	0.221377	0.145742	0.093812	0.066013	0.061691
0.4	0.464943	0.361215	0.271997	0.203595	0.163736	0.157421
0.5	0.580925	0.485240	0.397411	0.326053	0.282670	0.275732
0.6	0.671826	0.588998	0.510027	0.443744	0.402499	0.395866
0.7	0.742814	0.673611	0.606088	0.548312	0.511861	0.505974
0.8	0.798330	0.741726	0.685687	0.637159	0.606271	0.601263
0.9	0.841843	0.796161	0.750504	0.710658	0.685135	0.680982
1.0	0.876017	0.839471	0.802711	0.770458	0.749696	0.746303
1.1	0.902894	0.873832	0.844468	0.818601	0.801878	0.799130
1.2	0.924054	0.901043	0.877713	0.857097	0.843709	0.841495
1.3	0.940726	0.922567	0.904103	0.887740	0.877064	0.875285
1.4	0.953867	0.939577	0.925009	0.912062	0.903567	0.902138
1.5	0.964230	0.953014	0.941549	0.931329	0.924577	0.923427
1.6	0.972402	0.963623	0.954624	0.946571	0.941207	0.940279
1.7	0.978849	0.971999	0.964952	0.958619	0.954356	0.953604
1.8	0.983934	0.978610	0.973108	0.968136	0.964745	0.964134
1.9	0.987946	0.983827	0.979547	0.975652	0.972951	0.972450
2.0	0.991112	0.987945	0.984630	0.981585	0.979429	0.979016
2.1	0.993609	0.991194	0.988641	0.986268	0.984543	0.984199
2.2	0.995580	0.993758	0.991807	0.989964	0.988579	0.988289
2.3	0.997134	0.995781	0.994305	0.992881	0.991765	0.991518
2.4	0.998361	0.997377	0.996276	0.995183	0.994278	0.994066
2.5	0.999329	0.998636	0.997831	0.996999	0.996262	0.996076
2.6	1.000093	0.999630	0.999059	0.998432	0.997827	0.997662
2.7	1.000696	1.000415	1.000027	0.999563	0.999062	0.998914
2.8	1.001171	1.001033	1.000791	1.000456	1.000037	0.999902
2.9	1.001546	1.001522	1.001394	1.001160	1.000806	1.000681
3.0	1.001842	1.001907	1.001870	1.001715	1.001412	1.001296
3.1	1.002076	1.002211	1.002245	1.002154	1.001891	1.001781
3.2	1.002260	1.002451	1.002541	1.002500	1.002269	1.002164
3.3	1.002406	1.002640	1.002775	1.002773	1.002567	1.002466
3.4	1.002520	1.002789	1.002960	1.002988	1.002802	1.002705
3.5	1.002611	1.002907	1.003105	1.003158	1.002988	1.002893
3.6	1.002682	1.003000	1.003220	1.003292	1.003134	1.003041
3.7	1.002739	1.003073	1.003310	1.003398	1.003250	1.003158
3.8	1.002783	1.003131	1.003382	1.003481	1.003341	1.003251
3.9	1.002818	1.003177	1.003438	1.003547	1.003413	1.003324
4.0	1.002846	1.003213	1.003483	1.003599	1.003469	1.003381
4.1	1.002868	1.003241	1.003518	1.003640	1.003514	1.003427
4.2	1.002885	1.003264	1.003546	1.003672	1.003550	1.003462
4.3	1.002899	1.003282	1.003568	1.003698	1.003577	1.003491
4.4	1.002909	1.003296	1.003585	1.003718	1.003599	1.003513
4.5	1.002918	1.003307	1.003598	1.003734	1.003617	1.003531
4.6	1.002925	1.003315	1.003609	1.003746	1.003631	1.003544
4.7	1.002930	1.003322	1.003618	1.003756	1.003641	1.003555
4.8	1.002934	1.003328	1.003624	1.003764	1.003650	1.003564
4.9	1.002937	1.003332	1.003630	1.003770	1.003657	1.003571
5.0	1.002940	1.003335	1.003634	1.003775	1.003662	1.003576

CONCENTRATION PROFILES-ONE-DIMENSIONAL
HMC GENECUS MEDIUM

GRID POINTS

0.095240	0.190480	0.285720	0.380960	0.476200
0.571440	0.666680	0.761920	0.857160	0.952400
1.000000				

INITIAL CONDITION VECTOR

0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
0.0				

BOUNDARY CONDITION VECTOR

8.8053	C.C	C.C	0.0	0.0
0.0	0.0	0.0	0.0	0.0
C.C				

ORIGINAL COEFFICIENT MATRIX

25.6	-16.8	C.C	C.C	0.0	C.C	C.C	0.0	0.0	0.0	0.0
-27.3	44.1	-16.8	C.C	0.0	C.C	C.C	C.C	C.C	C.C	C.C
C.C	-27.3	44.1	-16.8	0.0	C.C	0.0	0.0	0.0	C.C	C.C
C.C	C.C	-27.3	44.1	-16.8	C.C	C.C	0.0	0.0	0.0	0.0
0.0	0.0	0.0	-27.3	44.1	-16.8	C.C	0.0	0.0	C.C	0.0
C.C	C.C	0.0	0.0	-27.3	44.1	-16.8	0.0	0.0	0.0	C.C
C.C	C.C	C.C	C.C	0.0	-27.3	44.1	-16.8	0.0	C.C	0.0
C.C	0.0	0.0	0.0	0.0	0.0	-27.3	44.1	-16.8	C.C	0.0
C.C	C.C	C.C	0.0	0.0	C.C	0.0	-27.3	44.1	-16.8	C.C
0.0	0.0	0.0	0.0	0.0	C.C	C.C	0.0	-36.4	88.2	-51.8
0.0	C.C	0.0	0.0	0.0	C.C	C.C	0.0	0.0	-176.4	176.4

MATRIX (C)

(CIAGCNAL ELEMENTS)

-1.0	1.3	-1.6	2.1	-2.6	3.4	-4.3	5.5	-7.0	10.3	-18.9
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ORIGINAL COEFFICIENT MATRIX

(CONVERTED INTO SYMMETRIC)

[illegible]

EIGENVALUES

1.868376	84.812375	4.698981	78.698066	20.190499
69.284016	10.865007	44.682663	31.829681	57.564572
238.491119				

EIGENVECTORS

0.287820	0.075696	-0.405584	-0.148577	0.409967
0.216372	0.425999	-0.331345	0.376345	-0.277608
0.000000				

-0.319049	0.209235	0.395988	-0.368277	-0.103738
0.441213	-0.293278	-0.295064	0.109289	-0.414180
0.000000				

0.341254	0.322049	-0.322858	-0.446363	-0.294169
0.302462	0.029070	0.323294	-0.438948	0.017194
0.000000				

-0.353807	0.402963	0.197927	-0.352809	0.432105
-0.085539	0.248172	0.303886	0.142149	0.424991
0.000001				

0.356354	0.443963	-0.041240	-0.123589	-0.188171
-0.403050	-0.414149	-0.315002	0.357522	0.250017
0.000011				

-0.348822	0.440988	-0.122064	0.153154	-0.222059
-0.388418	0.394448	-0.312481	-0.346945	-0.267795
0.000097				

0.331424	0.394331	0.265783	0.371005	0.436045
-0.053701	-0.197901	0.306475	-0.158784	-0.418391
0.000871				

-0.304652	0.308616	-0.366859	0.446193	-0.264679
0.325270	-0.087372	0.320844	0.437900	0.004733
0.007809				

0.269264	0.192331	0.409074	0.349807	-0.140596
0.436195	0.333473	-0.297720	-0.092053	0.421367
0.070001				

-0.195948	0.049359	-0.333988	0.102978	0.365134
0.162521	-0.372448	-0.284894	-0.333567	0.225339
0.543464				

C.107311	-0.051514	0.185924	-0.100747	-0.223421
-0.145025	C.215057	C.206740	C.220538	-0.181249
C.836472				

CHECK OF SIMILARITY TRANSFORMATION

25.610051	21.417811	-0.000000	-0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	-0.000000
C.000000				

21.417811	44.098236	21.417811	0.000000	-0.000000
-0.000000	-0.000000	-0.000000	-0.000000	0.000000
-0.000000				

-0.000000	21.417811	44.098236	21.417811	0.000000
0.000000	-0.000000	-0.000000	-0.000000	0.000000
0.000000				

-0.000000	0.000000	21.417811	44.098236	21.417811
0.000000	-0.000000	0.000000	0.000000	0.000000
-0.000000				

-0.000000	-0.000000	0.000000	21.417811	44.098236
21.417811	0.000000	0.000000	-0.000000	0.000000
C.000000				

-0.000000	-0.000000	0.000000	0.000000	21.417811
44.098236	21.417811	-0.000000	-0.000000	-0.000000
-0.000000				

-0.000000	-0.000000	-0.000000	-0.000000	0.000000
21.417811	44.098236	21.417811	0.000000	-0.000000
C.000000				

-0.000000	-0.000000	-0.000000	0.000000	0.000000
-0.000000	21.417811	44.098236	21.417811	-0.000000
-0.000000				

C.000000	-0.000000	-0.000000	0.000000	-0.000000
-0.000000	0.000000	21.417811	44.098236	24.731155
-0.000000				

-0.000000	0.000000	0.000000	0.000000	0.000000
-0.000000	-0.000000	-0.000000	24.731155	88.196472
95.578286				

0.000000	-0.000000	0.000000	-0.000000	0.000000
-0.000000	0.000000	-0.000000	-0.000000	95.578286
176.392944				

EIGENVALUES OF THE
ORIGINAL COEFFICIENT MATRIX

1.868376	84.812375	4.698981	78.698066	20.190499
69.284016	10.865007	44.682663	31.829681	57.564572
238.491119				

EIGENVECTORS OF THE
ORIGINAL COEFFICIENT MATRIX

-0.287820	-0.075696	0.405584	0.148577	-0.409967
-0.216372	-0.425999	0.331345	-0.376345	0.277608
-0.000000				

-0.406711	0.266725	0.504790	-0.469465	-0.132241
0.562441	-0.373860	-0.376136	0.139317	-0.527981
0.000000				

-0.554543	-0.523335	0.524649	0.725347	0.478030
-0.491506	-0.047239	-0.525358	0.713297	-0.027941
-0.000000				

-0.732914	0.834742	0.410007	-0.730846	0.895110
-0.177195	0.514090	0.629502	0.294463	0.880373
0.000003				

-0.941016	-1.172365	0.108902	0.326359	0.496899
1.064326	1.093634	0.831819	-0.944100	-0.660213
-0.000029				

-1.174216	1.484469	-0.410895	0.515553	-0.747502
-1.307508	1.327804	-1.051885	-1.167898	-0.901460
0.000327				

-1.422189	-1.692134	-1.140513	-1.592037	-1.871133
0.230440	0.849223	-1.315130	0.681367	1.795377
-0.003738				

-1.666506	1.688185	-2.006786	2.440761	-1.447842
1.779285	-0.477940	1.755076	2.395394	0.025893
0.042714				

-1.877630	-1.341157	-2.852549	-2.439268	0.980403
-3.041665	-2.325366	2.076059	0.641905	-2.938271
-0.488131				

-2.011265	0.506637	-3.428152	1.057001	3.747840
1.668167	-3.822915	-2.924242	-3.423830	2.312946

5.578277

-2.032623	0.975747	-3.521675	1.908306	4.231920
2.746997	-4.073499	-3.915956	-4.177327	3.433125
-15.844024				

SOLUTION OF THE DISPERSION MODELEQUATION

USING DANCKWERTS B.C.

SEMI-ANALYTICAL SOLUTION

STEP INPLT

CONCENTRATIONS AT GRID PCINTS					
TIME	1	2	3	4	5
C.C	C.CCCCCC	C.CC000C	0.0C0000	0.000000	C.000000
C.1	C.422828	C.2580C9	0.137772	C.064546	C.026697
0.2	0.593431	0.456549	0.328045	C.219383	C.136324
C.3	C.696657	C.587523	0.474474	0.365751	0.268485
0.4	C.766762	0.67966C	0.5844C9	0.486168	0.39C474
C.5	C.817199	0.747261	0.668C61	C.582679	0.494972
C.6	C.854797	C.7983C1	0.732738	C.659875	0.582306
0.7	0.883521	0.837651	0.783454	C.721892	0.65469C
C.8	C.9C5869	0.868479	0.823695	0.772001	C.714543
0.9	C.9235C3	0.892935	0.855936	C.8127C9	0.764020
1.C	0.937573	C.91253C	0.881969	0.845932	0.804937
1.1	C.948899	0.928355	0.9C3120	0.873148	0.838796
1.2	C.958C78	C.941215	C.92C388	C.895510	0.866830
1.3	0.965558	C.951715	0.934539	0.913925	0.89C050
1.4	C.971679	C.960322	0.94617C	0.929117	0.909291
1.5	C.976704	0.967396	C.95575C	C.941667	0.925239
1.6	C.98C84C	0.973223	C.963655	0.952045	0.938460
1.7	C.984251	C.978032	C.97C187	0.960634	0.949423
1.8	0.987C67	C.982005	C.975589	C.967745	0.958513
1.9	0.989396	0.985292	C.980C59	0.973637	0.966053
2.C	0.991322	C.988C12	C.983762	0.97852C	0.972306
2.1	0.992918	0.990264	0.986829	C.982567	C.977493
2.2	C.994239	0.992130	C.989371	0.985923	0.981795
2.3	C.995334	C.993677	C.991479	C.9887C5	C.985364
2.4	0.996241	0.994959	0.993226	C.991013	0.988324
2.5	C.996994	C.996C22	C.994675	C.992926	0.990780
2.6	0.997618	0.9969C3	0.995876	C.994514	0.992817
2.7	C.998135	0.997634	C.996873	0.995830	0.9945C6
2.8	C.998564	C.998241	C.997699	C.996923	0.995908
2.9	0.998920	C.998744	C.998385	C.997828	C.997C71
3.C	C.999215	0.999161	0.998953	0.998580	0.998036
3.1	C.99946C	C.9995C7	0.999425	0.999203	0.998836
3.2	C.999663	0.999794	0.999816	0.99972C	C.9995C0
3.3	C.999832	1.000032	1.000141	1.000149	1.000C51
3.4	C.999972	1.000229	1.00041C	1.000505	1.000508
3.5	1.000088	1.000393	1.000634	1.000801	1.000887
3.6	1.000184	1.000529	1.000819	1.001045	1.001201
3.7	1.000264	1.000642	1.000973	1.001249	1.001462
3.8	1.000330	1.000735	1.001100	1.001417	1.001679
3.9	1.000385	1.000813	1.0012C6	1.001557	1.001858
4.C	1.00043C	1.000877	1.001294	1.001673	1.002C07
4.1	1.000468	1.000931	1.001367	1.001769	1.002131
4.2	1.000499	1.000975	1.001427	1.001849	1.002233
4.3	1.000525	1.001012	1.001477	1.001915	1.002318
4.4	1.000547	1.001042	1.001519	1.001970	1.002389
4.5	1.000565	1.001067	1.001553	1.002C16	1.002447
4.6	1.000580	1.001088	1.001582	1.002C54	1.002496
4.7	1.000592	1.0011C6	1.0016C5	1.002C85	1.002536
4.8	1.0006C2	1.00112C	1.001625	1.002111	1.002569

4.9	1.000611	1.001132	1.001641	1.002133	1.002597	
5.0	1.000618	1.001142	1.001655	1.002150	1.002620	
CONCENTRATIONS AT GRID POINTS						
TIME	6	7	8	9	10	11
0.0	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.1	0.009825	0.003244	0.000968	0.000265	0.000080	0.000056
0.2	0.078695	0.042247	0.021168	0.010105	0.005348	0.004646
0.3	0.187411	0.124397	0.078875	0.049010	0.033518	0.031126
0.4	0.302399	0.225936	0.163869	0.118372	0.092642	0.088591
0.5	0.409185	0.329606	0.260519	0.206707	0.174877	0.169816
0.6	0.503340	0.426931	0.357806	0.302005	0.268142	0.262726
0.7	0.584383	0.514421	0.449429	0.395784	0.362710	0.357398
0.8	0.653264	0.591105	0.532333	0.483110	0.452445	0.447503
0.9	0.711373	0.657246	0.605442	0.561621	0.534121	0.529675
1.0	0.760162	0.713680	0.668807	0.630582	0.606461	0.602548
1.1	0.800993	0.761470	0.723074	0.690197	0.669358	0.665966
1.2	0.835087	0.801722	0.769157	0.741161	0.723347	0.720436
1.3	0.863508	0.835494	0.808051	0.784384	0.769269	0.766788
1.4	0.887170	0.863746	0.840733	0.820832	0.808074	0.805969
1.5	0.906854	0.887332	0.868105	0.851437	0.840711	0.838930
1.6	0.923216	0.906991	0.890974	0.877058	0.868063	0.866558
1.7	0.936811	0.923357	0.910048	0.898456	0.890927	0.889656
1.8	0.948101	0.936970	0.925935	0.916299	0.910003	0.908929
1.9	0.957476	0.948285	0.939154	0.931157	0.925896	0.924987
2.0	0.965258	0.957687	0.950145	0.943518	0.939122	0.938352
2.1	0.971717	0.965494	0.959278	0.953794	0.950121	0.949467
2.2	0.977078	0.971977	0.966865	0.962333	0.959263	0.958704
2.3	0.981526	0.977359	0.973165	0.969425	0.966856	0.966378
2.4	0.985216	0.981825	0.978395	0.975315	0.973162	0.972751
2.5	0.988279	0.985532	0.982736	0.980203	0.978398	0.978042
2.6	0.990819	0.988608	0.986338	0.984261	0.982744	0.982433
2.7	0.992927	0.991160	0.989328	0.987629	0.986350	0.986078
2.8	0.994676	0.993277	0.991809	0.990423	0.989343	0.989103
2.9	0.996127	0.995034	0.993867	0.992742	0.991827	0.991613
3.0	0.997330	0.996492	0.995575	0.994666	0.993887	0.993695
3.1	0.998329	0.997701	0.996991	0.996262	0.995597	0.995423
3.2	0.999157	0.998704	0.998167	0.997586	0.997016	0.996857
3.3	0.999845	0.999536	0.999142	0.998685	0.998193	0.998046
3.4	1.000415	1.000227	0.999951	0.999596	0.999169	0.999033
3.5	1.000888	1.000800	1.000622	1.000353	0.999979	0.999852
3.6	1.001280	1.001275	1.001179	1.000980	1.000651	1.000531
3.7	1.001605	1.001669	1.001641	1.001500	1.001208	1.001094
3.8	1.001875	1.001996	1.002024	1.001932	1.001671	1.001562
3.9	1.002099	1.002268	1.002342	1.002290	1.002055	1.001949
4.0	1.002285	1.002493	1.002606	1.002587	1.002373	1.002271
4.1	1.002439	1.002679	1.002825	1.002834	1.002637	1.002538
4.2	1.002567	1.002834	1.003006	1.003038	1.002856	1.002759
4.3	1.002673	1.002963	1.003157	1.003208	1.003038	1.002943
4.4	1.002761	1.003069	1.003282	1.003349	1.003188	1.003095
4.5	1.002834	1.003158	1.003385	1.003466	1.003313	1.003222
4.6	1.002895	1.003231	1.003471	1.003562	1.003417	1.003326
4.7	1.002945	1.003292	1.003543	1.003643	1.003503	1.003413
4.8	1.002987	1.003342	1.003602	1.003709	1.003575	1.003486
4.9	1.003021	1.003384	1.003651	1.003765	1.003634	1.003545
5.0	1.003050	1.003419	1.003692	1.003811	1.003683	1.003595


```

C      SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C      DIMENSIONAL HOMOGENEOUS CASE
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
      REAL*8  DX
      DOUBLE PRECISION  MATRIX(30,30),VECTOR(30,30)
      DOUBLE PRECISION X(30),VAR(30),CI(30),C1(30),
1TOLERC,W(30,30),CEVR(110,30),TIME(110),CUNC(110)
      DOUBLE PRECISION D(30,30),VICTOR(30,30)
C      READ THE DATA
      READ( 5,1)  N,NT
      READ(5,5)  ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 )  (X(J),J=1,N)
      READ( 5,2 )  (CI(J),J=1,N)
      READ(5,2)  (C1(J),J=1,N)
      READ(5,2)  (TIME(J), J=1,NT)
      READ(5,4) DX
      NORM=2
      TOLERC=0.000
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,220)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,223)
      WRITE(6,231)
      CALL LINECT(LINES,1,2)
      WRITE(6,232) (X(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,233)
      CALL LINECT(LINES,2,2)
      WRITE(6,234) (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,2,2)
      DO 30 J=1,N
30  C1(J)=C1(J)/(DX**2)
      WRITE(6,234) (C1(J),J=1,N)

```



```

CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,240)
DO 36 J=1,N
DO 36 K=1,N
  MATRIX(J,K)=MATRIX(J,K)/(DX**2)
36 CONTINUE
DO 31 J=1,N
  CALL LINECT(LINES,1,2)
31 WRITE(6,241) (MATRIX(J,K),K=1,N)
  CALL TRANS(N,DX,D,MATRIX)
  LINES=9
  WRITE(6,255)
  CALL LINECT(LINES,1,2)
  WRITE(6,241) (D(J,J),J=1,N)
  CALL LINECT(LINES,4,2)
  WRITE(6,223)
  WRITE(6,259)
  DO 50 J=1,N
    CALL LINECT(LINES,1,2)
50 WRITE(6,241) (MATRIX(J,K),K=1,N)
    CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NORM)
    WRITE(6,220)
    LINES =9
    CALL LINECT(LINES,3,2)
    WRITE(6,223)
    WRITE(6,242)
    CALL LINECT(LINES,2,2)
    WRITE(6,232) (MATRIX(J,J),J=1,N)
    CALL LINECT(LINES,3,2)
    WRITE(6,223)
    WRITE(6,243)
    DO 32 K=1,N
      CALL LINECT(LINES,4,2)
      WRITE(6,232) (VECTOR(K,J),J=1,N)
32 WRITE(6,223)
      CALL CHECK(VECTOR,MATRIX,N,W)
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,1,2)
      WRITE(6,244)
      DO 33 J=1,N
        CALL LINECT(LINES,4,2)
        WRITE(6,232) (W(J,K),K=1,N)
33 WRITE(6,223)
C   CALCULATE THE TRANSPOSE OF THE MATRIX OF
C   THE EIGENVECTORS
DO 40 I=1,N
DO 40 J=1,N
  VECTOR(I,J)=VECTOR(J,I)

```



```

40 CONTINUE
C   A=(D(-1)*A(*)*D)
C   A(*)=THE ORIGINAL COEFFICIENT MATRIX
C   D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C   OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C   A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C   COEFFICIENT MATRIX A(*)
C   Q=THE MATRIX OF EIGENVECTORS OF A
C   CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C   COEFFICIENT MATRIX
DO 38 I=1,N
DO 38 J=1,N
VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38 CONTINUE
WRITE(6,220)
LINES=9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,256)
CALL LINECT(LINES,2,2)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,257)
DO 39 K=1,N
CALL LINECT(LINES,3,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
39 WRITE(6,223)
C   (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
C   QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
C   D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
C   CALCULATE THE PRODUCT (QT*D(-1))
DO 41 I=1,N
DO 41 J=1,N
VICTOR(I,J)=VICTOR(I,J)/D(J,J)
41 CONTINUE
CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
ICEVR,VICTOR)
WRITE(6,223)
WRITE(6,225)
WRITE(6,245)
WRITE(6,223)
WRITE(6,264)
WRITE(6,223)
WRITE(6,246)
WRITE(6,248)
DO 34 JJ=2,NT
J=JJ-1
WRITE(6,251) TIME(JJ),(CEVR(J,K),K=1,5)
34 CONTINUE

```



```

WRITE(6,223)
WRITE(6,246)
WRITE(6,249)
DO 35 JJ=2,NT
J=JJ-1
WRITE(6,252) TIME(JJ), (CEVR(J,K),K=6,11 )
35 CONTINUE

```

C

FORMAT STATEMENTS

```

1  FORMAT(1X,2I4)
2  FORMAT(1CF8.5)
4  FORMAT(1X,F16.8)
5  FORMAT(11F7.4)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
111HDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
18HEQUATION/20X,19HUSING ORDINARY B.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,27HORIGIONAL COEFFICIENT MATRIX)
241 FORMAT(1H,10X,11F6.1)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME,9X,2H 6,8X,2H 7,8X,2H 8,
18X,2H 9, 8X, 2H10,8X,2H11)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
252 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
255 FORMAT(1H,10X,9HMATRIX(D)/10X,
119H(DIAGONAL ELEMENTS))
256 FORMAT(1H,20X,19H EIGENVALUES OF THE/20X,
127HORIGIONAL COEFFICIENT MATRIX)
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,
127HORIGIONAL COEFFICIENT MATRIX)
259 FORMAT(1H,30X,27HORIGIONAL COEFFICIENT MATRIX/
120X,26H(CONVERTED INTO SYMMETRIC))
264 FORMAT(1H,25X,18H SQUARE WAVE INPUT,
1/20X,26HC(0,THETA)=1 FOR 0<THETA<C,
2/20X,28HC(0,THETA)=-1 FOR C<THETA<2C)

```


F-25

STOP
END


```

SUBROUTINE SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME
1,NT,CEVR,VICTOR)

```

```

C
C THIS SUBROUTINE USES THE SEMI-ANALYTICAL SOLUTION
C TO EVALUATE THE CONCENTRATION PROFILES AT
C VARIOUS ELAPSED TIMES.
C

```

```

DOUBLE PRECISION VAR(30),VECTOR(30,30),C1(30),
1C1(30),MATRIX(30,30),TIME(110),CEVR(110,30),
2VICTOR(30,30)
3,CONST1(10,30),CONST2(10,30),ODD(20),EVEN(20)
DO 8 J=1,N
VAR(J)=0.0
DO 8 K=1,N
VAR(J)=VAR(J)+VICTOR(J,K)*C1(K)
8 CONTINUE
DO 9 J=1,N
C1(J)=VAR(J)
9 CONTINUE
DO 10 J=1,N
VAR(J)=0.0
DO 10 K=1,N
VAR(J)=VAR(J)+VICTOR(J,K)*C1(K)
10 CONTINUE
DO 11 J=1,N
EVEN(J)=0.0
11 C1(J)=VAR(J)
DO 50 I=1,5
DO 60 J=1,N
CONST1(I,J)=DEXP((-MATRIX(J,J))*(FLOAT(I)/10.))
CONST2(I,J)=1.-CONST1(I,J)
60 CONTINUE
50 CONTINUE
DO 51 JJ=1,5
DO 18 JK=1,6,5
DO 52 JL=1,5
L=JK+JL-1
DO 15 K=1,N
IF(L-5) 20,20,21
20 VAR(K)=EVEN(K)*CONST1(JL,K)+(MATRIX(K,K)*CONST1
1(JL,K)*C1(K)+CONST2(JL,K)*C1(K))/MATRIX(K,K)
IF(L-5) 15,30,15
30 ODD(K)=VAR(K)
GO TO 15
21 VAR(K)=ODD(K)*CONST1(JL,K)-(MATRIX(K,K)*CONST1
1(JL,K)*C1(K)+CONST2(JL,K)*C1(K))/MATRIX(K,K)
IF(L-10) 15,31,15
31 EVEN(K)=VAR(K)
15 CONTINUE
LL=(JJ-1)*10+L

```



```
DO 17 L1=1,N
CEVR(LL,L1)=0.0
DO 16 L2=1,N
16 CEVR(LL,L1)=CEVR(LL,L1)+VECTOR(L1,L2)*VAR(L2)
17 CONTINUE
52 CONTINUE
18 CONTINUE
51 CONTINUE
RETURN
END
```


SOLUTION OF THE DISPERSION MODELEQUATION
USING ORDINARY B.C.

SEMI-ANALYTICAL SOLUTION

SQUARE WAVE INPUT

$C(C, \text{THETA}) = 1$ FOR $0 < \text{THETA} < C$

$C(C, \text{THETA}) = -1$ FOR $C < \text{THETA} < 2C$

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.1	0.769229	0.510666	0.291627	0.144062	0.062142
0.2	0.331334	0.726742	0.556463	0.393956	0.257437
0.3	0.926401	0.825387	0.703163	0.570310	0.439045
0.4	0.950320	0.880262	0.791248	0.687711	0.576341
0.5	0.964789	0.914294	0.848165	0.768004	0.677251
0.6	-0.564208	-0.084435	0.303712	0.536548	0.627716
0.7	-0.781900	-0.500841	-0.198433	0.078167	0.293295
0.8	-0.367368	-0.685772	-0.471711	-0.243793	-0.027146
0.9	-0.711772	-0.788113	-0.632840	-0.455310	-0.268819
1.0	-0.938131	-0.849831	-0.735247	-0.598041	-0.445111
1.1	0.583373	0.131149	-0.220813	-0.409633	-0.450417
1.2	0.796063	0.535558	0.260613	0.018294	-0.156583
1.3	0.878043	0.713045	0.519076	0.317917	0.133311
1.4	0.919933	0.808254	0.669317	0.512744	0.351679
1.5	0.944431	0.865412	0.763556	0.642802	0.510009
1.6	-0.578475	-0.119019	0.242899	0.444661	0.501368
1.7	-0.792237	-0.525075	-0.243318	0.009135	0.196650
1.8	-0.375045	-0.705608	-0.505500	-0.296318	-0.101768
1.9	-0.917578	-0.802410	-0.658642	-0.495746	-0.326828
2.0	-0.942579	-0.860814	-0.755153	-0.629413	-0.490421
2.1	0.579934	0.122640	-0.236279	-0.434109	-0.485923
2.2	0.793386	0.523928	0.248536	-0.000365	-0.184469
2.3	0.875951	0.707658	0.509614	0.302879	0.111377
2.4	0.913292	0.804185	0.661387	0.500921	0.334408
2.5	0.943142	0.862213	0.757712	0.633495	0.496401
2.6	-0.579490	-0.121537	0.238298	0.437330	0.490641
2.7	-0.793036	-0.528058	-0.246943	0.003406	0.188192
2.8	-0.875674	-0.707171	-0.508358	-0.300874	-0.108440
2.9	-0.918074	-0.803642	-0.660396	-0.499339	-0.332091
3.0	-0.942970	-0.861785	-0.756930	-0.632247	-0.494573
3.1	0.579625	0.121874	-0.237681	-0.436345	-0.489198
3.2	0.793143	0.528324	0.247430	-0.002629	-0.187053
3.3	0.875759	0.707381	0.508742	0.301487	0.109338
3.4	0.918141	0.803808	0.661199	0.499823	0.332800
3.5	0.943023	0.861916	0.757169	0.632629	0.495132
3.6	-0.579584	-0.121771	0.237370	0.436646	0.489639
3.7	-0.793110	-0.528242	-0.247281	0.002366	0.187402
3.8	-0.875733	-0.707317	-0.508624	-0.301300	-0.109063
3.9	-0.918120	-0.803758	-0.661106	-0.499675	-0.332583
4.0	-0.943006	-0.861876	-0.757096	-0.632512	-0.494961
4.1	0.579597	0.121302	-0.237312	-0.436554	-0.489505
4.2	0.793120	0.528267	0.247327	-0.002704	-0.187295
4.3	0.875741	0.707336	0.508660	0.301357	0.109147
4.4	0.918126	0.803773	0.661134	0.499720	0.332649
4.5	0.943011	0.861888	0.757118	0.632548	0.495013
4.6	-0.579593	-0.121793	0.237830	0.436582	0.489546
4.7	-0.793117	-0.528260	-0.247313	0.002816	0.187328
4.8	-0.875738	-0.707330	-0.508649	-0.301340	-0.109122
4.9	-0.943015	-0.861878	-0.757126	-0.632606	-0.494929

5.0 -0.94321 -0.861885 -0.757112 -0.632537 -0.494997

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10	11
0.1	0.023652	0.008024	0.002450	0.000683	0.000209	0.000148
0.2	0.155311	0.086555	0.044915	0.022105	0.012004	0.010503
0.3	0.320263	0.221377	0.145742	0.093812	0.066013	0.061690
0.4	0.464943	0.361215	0.271997	0.203595	0.163736	0.157421
0.5	0.530925	0.485240	0.397411	0.326053	0.282670	0.275732
0.6	0.624523	0.572950	0.505128	0.442377	0.402082	0.395570
0.7	0.432192	0.500301	0.516258	0.504102	0.487853	0.484968
0.8	0.157805	0.298972	0.394204	0.449536	0.474244	0.477882
0.9	-0.038043	0.073731	0.206511	0.303469	0.357664	0.366139
1.0	-0.235834	-0.131010	0.007389	0.118351	0.184357	0.194838
1.1	-0.393455	-0.288116	-0.170687	-0.067521	-0.002704	0.007694
1.2	-0.250952	-0.272868	-0.244633	-0.195317	-0.156004	-0.149446
1.3	-0.015408	-0.118131	-0.175787	-0.198955	-0.203451	-0.203861
1.4	0.200067	0.069685	-0.032006	-0.102064	-0.139232	-0.144984
1.5	0.574047	0.244553	0.130949	0.042520	-0.009476	-0.017714
1.6	0.462963	0.377908	0.280843	0.195491	0.142033	0.133455
1.7	0.305746	0.343824	0.331871	0.296840	0.266651	0.261556
1.8	0.058617	0.174174	0.244793	0.279351	0.291132	0.292710
1.9	-0.165989	-0.025435	0.086544	0.165653	0.208615	0.215296
2.0	-0.347165	-0.209622	-0.087369	0.007736	0.064328	0.073302
2.1	-0.441755	-0.350337	-0.246826	-0.155793	-0.098697	-0.089536
2.2	-0.289015	-0.322065	-0.305017	-0.265494	-0.232428	-0.226871
2.3	-0.045416	-0.157004	-0.223596	-0.254606	-0.264112	-0.265326
2.4	0.176404	0.038984	-0.069815	-0.146122	-0.187288	-0.193680
2.5	0.355382	0.220314	0.101070	0.007678	-0.047495	-0.056242
2.6	0.448240	0.358774	0.257243	0.167958	0.111981	0.102999
2.7	0.294131	0.328722	0.313237	0.275093	0.242911	0.237495
2.8	0.049453	0.162256	0.230083	0.262180	0.272384	0.273710
2.9	-0.173219	-0.034340	0.074933	0.152099	0.193815	0.200296
3.0	-0.352369	-0.217044	-0.097032	-0.002962	0.052645	0.061462
3.1	-0.446257	-0.356194	-0.254057	-0.164236	-0.107917	-0.098880
3.2	-0.292566	-0.326686	-0.310723	-0.272157	-0.239704	-0.234245
3.3	-0.048218	-0.160650	-0.228099	-0.259863	-0.269354	-0.271145
3.4	0.174193	0.036107	-0.073368	-0.150271	-0.191819	-0.198272
3.5	0.353638	0.218044	0.098267	0.004405	-0.051070	-0.059866
3.6	0.445864	0.356983	0.255031	0.165375	0.109160	0.100140
3.7	0.293045	0.327309	0.311492	0.273055	0.240685	0.235239
3.8	0.048596	0.161141	0.228706	0.260572	0.270628	0.271930
3.9	-0.173895	-0.035720	0.073847	0.150830	0.192429	0.198891
4.0	-0.353403	-0.217738	-0.097889	-0.003963	0.051552	0.060354
4.1	-0.446573	-0.356741	-0.254733	-0.165026	-0.108730	-0.099755
4.2	-0.292898	-0.327119	-0.311257	-0.272780	-0.240385	-0.234935
4.3	-0.048480	-0.160991	-0.228520	-0.260355	-0.270391	-0.271690
4.4	0.173986	0.035838	-0.073700	-0.150659	-0.192242	-0.198702
4.5	0.353474	0.217832	0.098005	0.004098	-0.051404	-0.060205
4.6	0.445735	0.356315	0.254824	0.165133	0.108396	0.099873
4.7	0.292943	0.327177	0.311329	0.272864	0.240476	0.235028
4.8	0.048515	0.161037	0.228577	0.260421	0.270464	0.271763
4.9	-0.173958	-0.035302	0.073745	0.150711	0.192300	0.198760
5.0	-0.353452	-0.217603	-0.097969	-0.004057	0.051450	0.060250

SOLUTION OF THE DISPERSION MODELEQUATION
USING DANCKWERTS B.C.

SEMI-ANALYTICAL SOLUTION

SQUARE WAVE INPUT

$C(0, \theta) = 1$ FOR $0 < \theta < 0$

$C(0, \theta) = -1$ FOR $0 < \theta < 20$

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.1	0.422828	0.258009	0.137772	0.064546	0.026697
0.2	0.593431	0.456549	0.323045	0.219383	0.136324
0.3	0.696657	0.587523	0.474474	0.365751	0.268485
0.4	0.766762	0.679660	0.584409	0.486168	0.390473
0.5	0.817199	0.747261	0.668061	0.582679	0.494972
0.6	0.909141	0.822283	0.457194	0.530784	0.528911
0.7	-0.303341	-0.075447	0.127364	0.233126	0.382043
0.8	-0.487445	-0.306567	-0.125254	0.040500	0.177573
0.9	-0.610021	-0.466385	-0.312381	-0.159626	-0.016927
1.0	-0.656825	-0.581992	-0.454153	-0.319425	-0.185007
1.1	0.084960	-0.152229	-0.266811	-0.317510	-0.272421
1.2	0.377893	0.179011	0.009570	-0.109508	-0.169904
1.3	0.547134	0.389804	0.236097	0.101424	-0.002066
1.4	0.658196	0.533772	0.403114	0.276034	0.162199
1.5	0.735956	0.636857	0.527934	0.415160	0.305309
1.6	-0.053019	0.197096	0.347346	0.396407	0.372084
1.7	-0.351725	-0.142194	0.040228	0.174631	0.252497
1.8	-0.525624	-0.359514	-0.195048	-0.047604	0.070529
1.9	-0.640479	-0.508802	-0.369224	-0.231514	-0.105437
2.0	-0.721338	-0.616241	-0.499922	-0.378308	-0.258242
2.1	0.065097	-0.180056	-0.324173	-0.365884	-0.333052
2.2	0.361713	0.156292	-0.021044	-0.149342	-0.220124
2.3	0.533891	0.371185	0.210938	0.068563	-0.043679
2.4	0.647325	0.513469	0.382391	0.248890	0.127708
2.5	0.727009	0.624252	0.510635	0.392714	0.276715
2.6	-0.060396	0.186695	0.333219	0.377831	0.348376
2.7	-0.357817	-0.150788	0.028545	0.159250	0.232836
2.8	-0.530661	-0.366621	-0.204717	-0.060346	0.054224
2.9	-0.644647	-0.514685	-0.377232	-0.242074	-0.118961
3.0	-0.724788	-0.621113	-0.506556	-0.387061	-0.269459
3.1	0.062239	-0.184092	-0.329670	-0.373142	-0.342356
3.2	0.359345	0.152947	-0.025601	-0.155360	-0.227842
3.3	0.531928	0.368412	0.207159	0.063573	-0.050081
3.4	0.645698	0.516170	0.379256	0.244751	0.122397
3.5	0.725560	0.622346	0.508237	0.389281	0.272310
3.6	-0.061515	0.185114	0.331064	0.374984	0.344721
3.7	-0.358745	-0.152099	0.026758	0.156888	0.229804
3.8	-0.531430	-0.367709	-0.206200	-0.062305	0.051709
3.9	-0.645285	-0.515587	-0.378462	-0.243699	-0.121047
4.0	-0.725317	-0.621861	-0.507577	-0.388409	-0.271190
4.1	0.061799	-0.184712	-0.330517	-0.374260	-0.343792
4.2	0.358981	0.152433	-0.026303	-0.156238	-0.229033
4.3	0.531626	0.367985	0.206577	0.062803	-0.051069
4.4	0.645447	0.515816	0.378774	0.244113	0.121578
4.5	0.725452	0.622052	0.507836	0.388752	0.271630
4.6	-0.061688	0.184870	0.330732	0.374544	0.344157
4.7	-0.358888	-0.152302	0.026482	0.156523	0.229336
4.8	-0.531549	-0.367877	-0.206420	-0.062608	0.051320
4.9	-0.645383	-0.515726	-0.378652	-0.243950	-0.121369

5.0 -0.725399 -0.621977 -0.507734 -0.388617 -0.271457

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10	11
0.1	0.009825	0.003244	0.000968	0.000265	0.000080	0.000056
0.2	0.073695	0.042247	0.021168	0.010105	0.005348	0.004646
0.3	0.137411	0.124397	0.073875	0.049010	0.033518	0.031125
0.4	0.302399	0.225936	0.163869	0.118372	0.092642	0.088591
0.5	0.409185	0.329606	0.260519	0.206707	0.174877	0.169816
0.6	0.483689	0.420444	0.355869	0.301475	0.267983	0.262613
0.7	0.426993	0.429928	0.407093	0.375575	0.352015	0.348106
0.8	0.278442	0.342312	0.374583	0.385091	0.385409	0.385252
0.9	0.106575	0.205374	0.277704	0.324877	0.348837	0.352493
1.0	-0.058208	0.054468	0.147769	0.217167	0.256707	0.262916
1.1	-0.186036	-0.085905	0.009400	0.086717	0.133233	0.140627
1.2	-0.176290	-0.142626	-0.087366	-0.030198	0.008622	0.014932
1.3	-0.068199	-0.097923	-0.098865	-0.083817	-0.068585	-0.065966
1.4	0.069223	0.001126	-0.042413	-0.065667	-0.074884	-0.076198
1.5	0.204901	0.119184	0.051529	0.003687	-0.022457	-0.026535
1.6	0.303258	0.231425	0.158500	0.100144	0.065472	0.059965
1.7	0.278014	0.264261	0.228257	0.187494	0.158959	0.154288
1.8	0.152792	0.199399	0.216749	0.215732	0.209319	0.208108
1.9	0.001083	0.083412	0.140835	0.175992	0.192705	0.195216
2.0	-0.146496	-0.048830	0.030512	0.088393	0.120868	0.125958
2.1	-0.259757	-0.172921	-0.090196	-0.023407	0.016587	0.022944
2.2	-0.237747	-0.215640	-0.171440	-0.123617	-0.090623	-0.085240
2.3	-0.119368	-0.159010	-0.169520	-0.162605	-0.152465	-0.150658
2.4	0.026657	-0.049873	-0.101594	-0.131834	-0.145438	-0.147453
2.5	0.169516	0.076675	0.002079	-0.051707	-0.081593	-0.086268
2.6	0.278859	0.196034	0.117256	0.053874	0.016035	0.010022
2.7	0.253596	0.234823	0.193903	0.148912	0.117710	0.112613
2.8	0.132519	0.174929	0.188164	0.183602	0.174952	0.173383
2.9	-0.015747	0.063081	0.117066	0.149261	0.164103	0.166315
3.0	-0.160465	-0.065715	0.010760	0.066170	0.097083	0.101922
3.1	-0.271350	-0.186941	-0.106603	-0.041873	-0.003181	0.002968
3.2	-0.247366	-0.227278	-0.165064	-0.138955	-0.107045	-0.101835
3.3	-0.127350	-0.168669	-0.180830	-0.175340	-0.166103	-0.164440
3.4	0.020035	-0.057889	-0.110982	-0.142407	-0.156760	-0.153895
3.5	0.164022	0.070023	-0.005712	-0.060483	-0.090991	-0.095766
3.6	0.274300	0.190515	0.110790	0.046591	0.008235	0.002140
3.7	0.249814	0.230243	0.188538	0.142869	0.111237	0.106072
3.8	0.129361	0.171129	0.183712	0.178588	0.169581	0.167955
3.9	-0.018350	0.059929	0.113373	0.145101	0.159646	0.161811
4.0	-0.162624	-0.068330	0.007696	0.062718	0.093385	0.093185
4.1	-0.273141	-0.189111	-0.109145	-0.044737	-0.006249	-0.000133
4.2	-0.248852	-0.229078	-0.187173	-0.141331	-0.109590	-0.104407
4.3	-0.128583	-0.170163	-0.182580	-0.177312	-0.168214	-0.166574
4.4	0.019012	-0.059127	-0.112433	-0.144042	-0.158512	-0.160665
4.5	0.163173	0.068995	-0.006917	-0.061840	-0.092444	-0.097235
4.6	0.273597	0.189663	0.109791	0.045466	0.007029	0.000921
4.7	0.249230	0.229536	0.187710	0.141935	0.110237	0.105061
4.8	0.128896	0.170542	0.183025	0.177813	0.168751	0.167117
4.9	-0.018752	0.059442	0.112803	0.144458	0.158958	0.161115
5.0	-0.162957	-0.068734	0.007223	0.062185	0.092814	0.097608


```

C      SOLUTION OF THE DISPERSION MODEL EQUATION-ONE
C      DIMENSIONAL HOMOGENEOUS CASE
C      INPUT DATA
C      N= THE NUMBER OF GRID POINTS.
C      NT = THE TOTAL NO. OF TIMES.
C      MATRIX=THE COEFFICIENT MATRIX
C      X= THE DIMENSIONLESS DISTANCES OF GRID POINTS.
C      CI= THE INITIAL CONDITION VECTOR.
C      C1= THE BOUNDARY CONDITION VECTOR.
C      TIME= THE DIMENSIONLESS TIMES.
C      DX= THE GRID SPACING.
      REAL*8 DX,W1,BB,BB1
      DOUBLE PRECISION MATRIX(30,30),VECTOR(30,30)
      DOUBLE PRECISION X(30),VAR(30),CI(30),C1(30),
      ITOLERC,W(30,30),CEVR(110,30),TIME(110),CUNC(110)
      DOUBLE PRECISION D(30,30),VICTOR(30,30)
C      READ THE DATA
      READ( 5,1)  N,NT
      READ(5,5)  ((MATRIX(I,J),J=1,N),I=1,N)
      READ( 5,2 )  (X(J),J=1,N)
      READ( 5,2 )  (CI(J),J=1,N)
      READ( 5,2 )  (C1(J),J=1,N)
      READ(5,2)  (TIME(J), J=1,NT)
      READ(5,4) DX
      NORM=2
      TOLERC=0.000
      WRITE(6,223)
      LINES=9
      CALL LINECT(LINES,4,2)
      WRITE(6,253) DX
      WRITE(6,220)
      LINES =9
      CALL LINECT(LINES,4,2)
      WRITE(6,224)
      WRITE(6,223)
      WRITE(6,231)
      CALL LINECT(LINES,1,2)
      WRITE(6,232) (X(J),J=1,N)
      CALL LINECT(LINES,4,2)
      WRITE(6,223)
      WRITE(6,233)
      CALL LINECT(LINES,2,2)
      WRITE(6,234) (CI(J),J=1,N)
      CALL LINECT(LINES,4,2)
      DO 30 J=1,N
30  CI(J)=C1(J)/(DX**2)
      WRITE(6,223)
      WRITE(6,235)
      CALL LINECT(LINES,2,2)
      WRITE(6,267)

```



```

WRITE(6,234) (C1(J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,240)
DO 35 J=1,N
DO 36 K=1,N
MATRIX(J,K)=MATRIX(J,K)/(DX**2)
36 CONTINUE
DO 31 J=1,N
CALL LINECT(LINES,1,2)
31 WRITE(6,241)(MATRIX(J,K),K=1,N)
CALL TRANS(N,DX,D,MATRIX)
LINES=9
WRITE(6,255)
CALL LINECT(LINES,1,2)
WRITE(6,241) (D(J,J),J=1,N)
CALL LINECT(LINES,4,2)
WRITE(6,223)
WRITE(6,259)
DO 50 J=1,N
CALL LINECT(LINES,1,2)
50 WRITE(6,241) (MATRIX(J,K),K=1,N)
CALL JACOBI(N,MATRIX, VECTOR,TOLERC,NDRM)
WRITE(6,220)
LINES =9
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,242)
CALL LINECT(LINES,2,2)
WRITE(6,232) (MATRIX(J,J),J=1,N)
CALL LINECT(LINES,3,2)
WRITE(6,223)
WRITE(6,243)
DO 32 K=1,N
CALL LINECT(LINES,4,2)
WRITE(6,232) (VECTOR(K,J),J=1,N)
32 WRITE(6,223)
CALL CHECK(VECTOR,MATRIX,N,W)
WRITE(6,220)
LINES=9
CALL LINECT(LINES,1,2)
WRITE(6,244)
DO 33 J=1,N
CALL LINECT(LINES,4,2)
WRITE(6,232) (w(J,K),K=1,N)
33 WRITE(6,223)
C CALCULATE THE TRANSPOSE OF THE MATRIX OF
C THE EIGENVECTORS
DO 40 I=1,N
DO 40 J=1,N

```



```

      VECTOR(I,J)=VECTOR(J,I)
40  CONTINUE
C    A=D(-1)*A(*)*D)
C    A(*)=THE ORIGINAL COEFFICIENT MATRIX
C    D=THE DIAGONAL MATRIX USED FOR THE CONVERSION
C    OF MATRIX (A(*)) TO THE SYMMETRIC FORM
C    A=THE SYMMETRIC MATRIX DERIVED FROM THE ORIGINAL
C    COEFFICIENT MATRIX A(*)
C    Q=THE MATRIX OF EIGENVECTORS OF A
C    CALCULATE THE EIGENVECTORS OF THE ORIGINAL
C    COEFFICIENT MATRIX
      DO 38 I=1,N
      DO 38 J=1,N
      VECTOR(I,J)=D(I,I)*VECTOR(I,J)
38  CONTINUE
      WRITE(6,220)
      LINES=9
      CALL LINECT(LINES,3,2)
      WRITE(6,223)
      WRITE(6,256)
      CALL LINECT(LINES,2,2)
      WRITE(6,232) (MATRIX(J,J),J=1,N)
      CALL LINECT(LINES,3,2)
      WRITE(6,223)
      WRITE(6,257)
      DO 39 K=1,N
      CALL LINECT(LINES,3,2)
      WRITE(6,232) (VECTOR(K,J),J=1,N)
39  WRITE(6,223)
C    (D*Q)(-1)= Q(-1)*D(-1)=QT*D(-1)
C    QT=THE TRANSPOSE OF THE MATRIX OF EIGENVECTORS OF A
C    D(-1)=THE INVERSE OF MATRIX D AS DEFINED PREVIOUSLY
C    CALCULATE THE PRODUCT (QT*D(-1))
      DO 41 I=1,N
      DO 41 J=1,N
      VECTOR(I,J)=VECTOR(I,J)/D(J,J)
41  CONTINUE
      CALL SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME,NT,
1CEVR,VECTOR)
      WRITE(6,223)
      WRITE(6,225)
      WRITE(6,245)
      WRITE(6,223)
      WRITE(6,264)
      WRITE(6,223)
      WRITE(6,245)
      WRITE(6,248)
      DO 34 J=1,NT
34  WRITE(6,251) TIME(J), (CEVR(J,K),K=1,5)
      WRITE(6,223)

```



```

WRITE(6,245)
WRITE(6,249)
DO 35 J=1,NT
35 WRITE(6,252) TIME(J), (CEVR(J,K),K=6,11)
W1=10.0
BB=0.25
BB1=0.75
DO 51 J=1,NT
CONC(J)=BB*SIN(W1*TIME(J))+BB1
51 CONTINUE
WRITE(6,220)
WRITE(6,223)
WRITE(6,263)
DO 52 J=1,NT
WRITE(6,269) TIME(J), CONC(J), CEVR(J,11)
52 CONTINUE

```

C FORMAT STATEMENTS

```

1  FORMAT(1X,214)
2  FORMAT(10F8.5)
4  FORMAT(1X,F15.8)
5  FORMAT(11F7.4)
220 FORMAT(1H2)
221 FORMAT(1H,10X,8H ..CONTD)
222 FORMAT(1H,/)
223 FORMAT(1H,/)
224 FORMAT(1H,18X,28H CONCENTRATION PROFILES-ONE-,
111NDIMENSIONAL/25X,22H HOMOGENEOUS MEDIUM)
225 FORMAT(1H,20X,32HSOLUTION OF THE DISPERSION MODEL,
18HEQUATION/20X,19HUSING ORDINARY O.C.)
231 FORMAT(1H,30X,12H GRID POINTS)
232 FORMAT(1H,10X,5F11.6)
233 FORMAT(1H,30X,25H INITIAL CONDITION VECTOR)
234 FORMAT(1H,10X,5F12.4)
235 FORMAT(1H,30X,26H BOUNDARY CONDITION VECTOR)
240 FORMAT(1H,30X,27H ORIGINAL COEFFICIENT MATRIX)
241 FORMAT(1H,10X,11F6.1)
242 FORMAT(1H,30X,12H EIGENVALUES)
243 FORMAT(1H,30X,13H EIGENVECTORS)
244 FORMAT(1H,20X,35H CHECK OF SIMILARITY TRANSFORMATION)
245 FORMAT(1H,30X,25H SEMI-ANALYTICAL SOLUTION)
246 FORMAT(1H,25X,29HCONCENTRATIONS AT GRID POINTS)
248 FORMAT(1H,15X, 5H TIME, 5X, 2H 1, 9X, 2H 2, 8X,
12H 3, 8X, 2H 4, 8X, 2H 5)
249 FORMAT(1H,15X, 5H TIME, 9X, 2H 6, 8X, 2H 7, 8X, 2H 8,
18X, 2H 9, 8X, 2H 10, 8X, 2H 11)
251 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
252 FORMAT(1H, 15X, F6.1, 2X, 5F10.6)
253 FORMAT(1H,10X,13HGRID SPACING=, F11.6)
255 FORMAT(1H,10X,29HMATRIX(D)/10X,
119H(DIAGONAL ELEMENTS))

```



```
256 FORMAT(1H,27X,19H EIGENVALUES OF THE/20X,  
127HORIGINAL COEFFICIENT MATRIX)  
257 FORMAT(1H,20X,20H EIGENVECTORS OF THE/20X,  
127HORIGINAL COEFFICIENT MATRIX)  
259 FORMAT(1H,30X,27HORIGINAL COEFFICIENT MATRIX/  
120X,25H(CONVERTED INTO SYMMETRIC))  
264 FORMAT(1H,40X,17H SINUSOIDAL INPUT,  
1/30X,21HC(0,Q)=0.75+0.25SINWQ)  
267 FORMAT(1H,10X,30HS(U)=0.24762(0.25SIN(WQ)+0.75))  
268 FORMAT(1H,10X,5H TIME,10X,12HINPUT SIGNAL,  
110X,14H OUTPUT SIGNAL)  
269 FORMAT(1H,10X,F6.1,10X,F12.6,10X,F12.6)  
STOP  
END
```



```

SUBROUTINE SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME
1,NT,CEVR,VICTOR)

```

```

C
C THIS SUBROUTINE USES THE SEMI-ANALYTICAL SOLUTION
C TO EVALUATE THE CONCENTRATION PROFILES AT
C VARIOUS ELAPSED TIMES.
C

```

```

REAL*8 CONST,W,B1,B2,B3, CONST1,CONST2,
1CONST3,CONST4,CONST5
DOUBLE PRECISION VAR(30),VECTOR(30,30),C1(30),
1C1(30),MATRIX(30,30),TIME(110),CEVR(110,30),
2VICTOR(30,30)
DO 8 J=1,N
VAR(J)=0.0
DO 8 K=1,N
VAR(J)=VAR(J)+VICTOR(J,K)*C1(K)
8 CONTINUE
DO 9 J=1,N
9 C1(J)=VAR(J)
DO 10 J=1,N
VAR(J)=0.0
DO 10 K=1,N
VAR(J)=VAR(J)+VICTOR(J,K)*C1(K)
10 CONTINUE
DO 11 J=1,N
11 C1(J)=VAR(J)
DO 18 J=1,NT
DO 15 K=1,N
W=10.0
B1=0.25
B2=0.75
B3=1.0
CONST=-MATRIX(K,K)*TIME(J)
CONST1=MATRIX(K,K)/W
CONST2=B2/MATRIX(K,K)
CONST3=B1/(B3+CONST1**2)
CONST4=CONST3*((CONST1/W)*SIN(W*TIME(J))
1-(B3/W)*COS(W*TIME(J)))+CONST2
CONST5=(CONST3/W)-CONST2
15 VAR(K)=(DEXP(CONST)*C1(K)+ C1(K)*CONST4
1+(DEXP(CONST)*C1(K))*CONST5)
DO 17 L1=1,N
CEVR(J,L1)=0.0
DO 16 L2=1,N
16 CEVR(J,L1)=CEVR(J,L1)+VECTOR(L1,L2)*VAR(L2)
17 CONTINUE
18 CONTINUE
RETURN
END

```


AM INTERRUPT() OLD PSW IS FF25000D9202429A
 AM INTERRUPT() OLD PSW IS FF25000DA202428A
 AM INTERRUPT() OLD PSW IS FF25000D9202429E
 AM INTERRUPT() OLD PSW IS FF25000DA202428A
 AM INTERRUPT() OLD PSW IS FF25000DA202429E

SOLUTION OF THE DISPERSION MODELEQUATION
 USING ORDINARY B.C.
 SEMI-ANALYTICAL SOLUTION

SINUSOIDAL INPUT
 $C(0,Q)=0.75+0.25\sin Q$

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.750000	0.750000	0.750000	0.750000	0.750000
0.1	0.871883	0.811886	0.777841	0.761294	0.754286
0.2	0.949547	0.901920	0.853672	0.814534	0.787087
0.3	0.860294	0.886386	0.880489	0.858247	0.831199
0.4	0.677405	0.762873	0.814214	0.836491	0.838156
0.5	0.565768	0.637982	0.705959	0.758535	0.792308
0.6	0.626444	0.623005	0.649824	0.689322	0.728801
0.7	0.802772	0.720694	0.694171	0.688160	0.701044
0.8	0.932107	0.858716	0.796157	0.752231	0.731004
0.9	0.895197	0.890635	0.860631	0.822709	0.788553
1.0	0.725745	0.795549	0.827352	0.831285	0.818866
1.1	0.579382	0.660484	0.726222	0.770023	0.792629
1.2	0.590556	0.609331	0.649706	0.694459	0.732859
1.3	0.748905	0.688904	0.667767	0.673465	0.692655
1.4	0.908778	0.825881	0.763504	0.725882	0.710399
1.5	0.923138	0.894200	0.848671	0.803158	0.767178
1.6	0.773742	0.830952	0.844787	0.833967	0.811385
1.7	0.608318	0.694211	0.755286	0.789765	0.802056
1.8	0.568528	0.609637	0.662347	0.711018	0.747519
1.9	0.695936	0.654940	0.651332	0.669991	0.697717
2.0	0.873390	0.783432	0.732302	0.704298	0.698282
2.1	0.937727	0.887353	0.830760	0.782313	0.748573
2.2	0.829787	0.860732	0.856144	0.832244	0.802255
2.3	0.643303	0.733027	0.785083	0.808132	0.809897
2.4	0.561164	0.621635	0.632384	0.732104	0.764413
2.5	0.647441	0.628959	0.643488	0.674029	0.707574
2.6	0.828308	0.743255	0.703100	0.687274	0.691599
2.7	0.937473	0.869838	0.806900	0.759642	0.731146
2.8	0.874569	0.891918	0.859445	0.824582	0.789833
2.9	0.697427	0.773385	0.812417	0.822376	0.813635
3.0	0.568910	0.644021	0.709048	0.755043	0.780757
3.1	0.607174	0.612759	0.644369	0.684479	0.721313
3.2	0.777039	0.703339	0.677843	0.675556	0.689995
3.3	0.922331	0.842884	0.778690	0.736472	0.715591
3.4	0.909469	0.892693	0.854190	0.811217	0.774561
3.5	0.750277	0.811969	0.834926	0.831063	0.812685
3.6	0.591116	0.674930	0.738609	0.777772	0.794908
3.7	0.578318	0.607568	0.653790	0.700327	0.737571
3.8	0.723648	0.671815	0.658451	0.669934	0.693388
3.9	0.803491	0.808602	0.748306	0.714535	0.702978

4.1	0.803133	0.845581	0.857773	0.833445	0.806874
4.2	0.626006	0.711883	0.759177	0.798427	0.805656
4.3	0.563163	0.613785	0.670072	0.720265	0.754989
4.4	0.672382	0.641579	0.646447	0.670820	0.701455
4.5	0.853246	0.769710	0.718150	0.695551	0.694273
4.6	0.959471	0.880376	0.820153	0.771721	0.740045
4.7	0.851781	0.871831	0.858684	0.829298	0.796689
4.8	0.670799	0.751930	0.798308	0.815347	0.812126
4.9	0.562918	0.630911	0.694539	0.742694	0.772164
5.0	0.627323	0.620037	0.642782	0.678135	0.713543

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10	11
0.0	0.750000	0.750000	0.750000	0.750000	0.750000	0.750000
0.1	0.751664	0.750782	0.750493	0.750347	0.750148	0.750066
0.2	0.769911	0.750148	0.755037	0.752527	0.751366	0.751144
0.3	0.806258	0.786504	0.772495	0.763562	0.758933	0.758172
0.4	0.827819	0.812478	0.796982	0.784367	0.776767	0.775510
0.5	0.808956	0.812762	0.808788	0.801876	0.796353	0.795385
0.6	0.760936	0.782994	0.795527	0.800973	0.802341	0.802451
0.7	0.722884	0.746137	0.766118	0.780518	0.788206	0.789350
0.8	0.725849	0.732108	0.743925	0.756112	0.764126	0.765373
0.9	0.764052	0.750451	0.745878	0.746740	0.748849	0.749187
1.0	0.790998	0.781546	0.767133	0.757790	0.753104	0.752342
1.1	0.798791	0.794573	0.785595	0.776285	0.770013	0.768049
1.2	0.760095	0.775758	0.782174	0.782853	0.781504	0.781183
1.3	0.718354	0.740994	0.758313	0.769512	0.774921	0.775693
1.4	0.711053	0.721088	0.734578	0.746953	0.754613	0.755791
1.5	0.744204	0.733455	0.731698	0.734653	0.737831	0.738393
1.6	0.736777	0.765012	0.751450	0.742911	0.739010	0.738382
1.7	0.799194	0.783265	0.774985	0.763334	0.756090	0.754885
1.8	0.769693	0.779311	0.780118	0.776509	0.772724	0.772026
1.9	0.725135	0.747030	0.761698	0.769819	0.773070	0.773489
2.0	0.706265	0.720825	0.736319	0.749017	0.756375	0.757490
2.1	0.730267	0.724570	0.727045	0.732914	0.737645	0.738389
2.2	0.774942	0.754649	0.742169	0.736066	0.733829	0.733473
2.3	0.790111	0.783272	0.767660	0.755379	0.748222	0.747045
2.4	0.780470	0.784015	0.779907	0.772942	0.767420	0.766455
2.5	0.736093	0.756110	0.767566	0.772485	0.773641	0.773722
2.6	0.706728	0.725147	0.741900	0.754332	0.761059	0.762059
2.7	0.719333	0.719539	0.726442	0.735097	0.741159	0.742104
2.8	0.762286	0.744401	0.735351	0.732404	0.732171	0.732137
2.9	0.796072	0.775842	0.760397	0.748682	0.742307	0.741269
3.0	0.789608	0.787010	0.778520	0.768927	0.762208	0.761064
3.1	0.748821	0.765536	0.773033	0.774497	0.773543	0.773283
3.2	0.711198	0.732147	0.748960	0.760248	0.765867	0.766673
3.3	0.711320	0.717528	0.728419	0.739260	0.746217	0.747290
3.4	0.749067	0.735110	0.730282	0.730817	0.732642	0.732934
3.5	0.789728	0.766719	0.752826	0.742669	0.737612	0.736795
3.6	0.795915	0.787450	0.775318	0.763910	0.756547	0.755314
3.7	0.761937	0.774076	0.777071	0.775005	0.772030	0.771457
3.8	0.719028	0.740890	0.756470	0.765747	0.769821	0.770375
3.9	0.706638	0.718399	0.732451	0.744643	0.751945	0.753059
4.0	0.735155	0.727280	0.727094	0.731094	0.734834	0.735424
4.1	0.780441	0.759365	0.745322	0.737552	0.734216	0.733662
4.2	0.798777	0.785154	0.770374	0.758079	0.750658	0.749431
4.3	0.774305	0.780936	0.779217	0.773800	0.769040	0.768190
4.4	0.729524	0.750587	0.763718	0.770260	0.772461	0.772711
4.5	0.705604	0.722010	0.738127	0.750713	0.757775	0.758835
4.6	0.724537	0.721477	0.725971	0.733129	0.738483	0.739320
4.7	0.763916	0.749478	0.738426	0.733674	0.732321	0.732107
4.8	0.797939	0.780269	0.764040	0.751847	0.744954	0.743826
4.9	0.784921	0.785540	0.779264	0.770939	0.764767	0.763704
5.0	0.741832	0.760445	0.770100	0.773396	0.773543	0.773463

ME	INPUT SIGNAL	OUTPUT SIGNAL
0.0	0.750000	0.750000
0.1	0.960368	0.750056
0.2	0.977324	0.751144
0.3	0.755280	0.758172
0.4	0.550799	0.775510
0.5	0.510269	0.795385
0.6	0.680146	0.802451
0.7	0.914247	0.789350
0.8	0.997340	0.765373
0.9	0.853030	0.749187
1.0	0.613995	0.752342
1.1	0.500002	0.768949
1.2	0.615857	0.781188
1.3	0.855042	0.775693
1.4	0.997652	0.755791
1.5	0.912572	0.738393
1.6	0.678024	0.738332
1.7	0.509651	0.754885
1.8	0.562253	0.772026
1.9	0.767469	0.773489
2.0	0.978236	0.757490
2.1	0.959164	0.738389
2.2	0.747787	0.733473
2.3	0.538445	0.747045
2.4	0.523605	0.766455
2.5	0.716912	0.773722
2.6	0.940640	0.762059
2.7	0.989094	0.742104
2.8	0.817726	0.732137
2.9	0.584092	0.741269
3.0	0.502992	0.761064
3.1	0.648991	0.773288
3.2	0.887857	0.766678
3.3	0.999978	0.747290
3.4	0.882271	0.732934
3.5	0.642954	0.736795
3.6	0.502055	0.755314
3.7	0.589115	0.771457
3.8	0.824092	0.770375
3.9	0.990949	0.753059
4.0	0.936273	0.735424
4.1	0.710344	0.733682
4.2	0.520870	0.749431
4.3	0.542056	0.768190
4.4	0.754425	0.772711
4.5	0.962726	0.758835
4.6	0.975447	0.739320
4.7	0.730893	0.732107
4.8	0.557936	0.743826
4.9	0.511562	0.763704
5.0	0.684400	0.773463

AM INTERRUPT ()	CLD	PSW	IS	FF25000D9202429A
AM INTERRUPT ()	CLD	PSW	IS	FF25000DA202428A
AM INTERRUPT ()	CLD	PSW	IS	FF25000D9202429E
AM INTERRUPT ()	CLD	PSW	IS	FF25000DA202428A
AM INTERRUPT ()	CLD	PSW	IS	FF25000D9202429E
AM INTERRUPT ()	CLD	PSW	IS	FF25000DA202428A
AM INTERRUPT ()	CLD	PSW	IS	FF25000DA202429E
AM INTERRUPT ()	CLD	PSW	IS	FF25000DA202428A
AM INTERRUPT ()	CLD	PSW	IS	FF25000DA202429E

SOLUTION OF THE DISPERSION MODELEQUATION
USING DANCKWERTS B.C.
SEMI-ANALYTICAL SOLUTION

SINUSOIDAL INPUT
 $C(\theta, Q) = 0.75 + 0.25 \sin \omega Q$

CONCENTRATIONS AT GRID POINTS

TIME	1	2	3	4	5
0.0	0.750000	0.750000	0.750000	0.750000	0.750000
0.1	0.808216	0.778163	0.762276	0.754960	0.751992
0.2	0.872871	0.836664	0.805861	0.783318	0.768587
0.3	0.856058	0.852907	0.837269	0.816944	0.797476
0.4	0.760347	0.800165	0.818233	0.820429	0.813031
0.5	0.669990	0.719911	0.759220	0.784877	0.797719
0.6	0.663446	0.681351	0.709429	0.738123	0.761721
0.7	0.744311	0.716786	0.710959	0.719301	0.734552
0.8	0.836537	0.791363	0.759679	0.742698	0.738137
0.9	0.854096	0.834897	0.808739	0.784432	0.766636
1.0	0.779922	0.806072	0.811452	0.804256	0.791747
1.1	0.681507	0.730448	0.764089	0.782446	0.788651
1.2	0.648791	0.676805	0.709223	0.737847	0.758764
1.3	0.711424	0.693370	0.696519	0.710487	0.728386
1.4	0.811482	0.765421	0.737031	0.724725	0.724471
1.5	0.856700	0.825419	0.793006	0.766820	0.749812
1.6	0.805284	0.813269	0.812567	0.797536	0.780443
1.7	0.704327	0.750353	0.777391	0.788194	0.787650
1.8	0.646501	0.683907	0.719542	0.747020	0.764348
1.9	0.684852	0.679853	0.691977	0.711571	0.731582
2.0	0.784021	0.741778	0.719851	0.714191	0.719162
2.1	0.852751	0.812635	0.777381	0.752267	0.738246
2.2	0.827785	0.827183	0.811546	0.790622	0.771072
2.3	0.732022	0.771968	0.790828	0.793853	0.787281
2.4	0.653459	0.697691	0.734187	0.758873	0.771821
2.5	0.664289	0.672587	0.693626	0.717746	0.738783
2.6	0.754524	0.719693	0.706375	0.708204	0.718440
2.7	0.841176	0.795663	0.760663	0.738954	0.729409
2.8	0.844555	0.830620	0.806536	0.781670	0.761536
2.9	0.761538	0.792399	0.801785	0.797033	0.785225
3.0	0.663434	0.716120	0.750748	0.770881	0.778648
3.1	0.650821	0.671895	0.700326	0.727227	0.747811

3.3	0.822529	0.775354	0.743513	0.727069	0.722906
3.4	0.853967	0.827896	0.797386	0.775671	0.751684
3.5	0.790286	0.809682	0.808934	0.796883	0.780891
3.6	0.690039	0.737450	0.757530	0.781595	0.783657
3.7	0.645369	0.677605	0.711233	0.738850	0.757427
3.8	0.607738	0.685164	0.691796	0.707941	0.726305
3.9	0.794216	0.753172	0.727084	0.717278	0.718896
4.0	0.855180	0.819101	0.784649	0.758270	0.742004
4.1	0.815901	0.822333	0.811562	0.793226	0.774377
4.2	0.716490	0.759894	0.783077	0.790002	0.786247
4.3	0.648344	0.689169	0.725380	0.751560	0.766696
4.4	0.674115	0.675222	0.691515	0.713240	0.733696
4.5	0.770108	0.730832	0.712616	0.710271	0.717584
4.6	0.843067	0.804892	0.769281	0.745381	0.733170
4.7	0.836316	0.829309	0.809412	0.786288	0.766124
4.8	0.745658	0.781634	0.796111	0.795381	0.786145
4.9	0.659444	0.705699	0.741607	0.764299	0.774825
5.0	0.656937	0.671317	0.696009	0.721618	0.742570

CONCENTRATIONS AT GRID POINTS

TIME	6	7	8	9	10	11
0.0	0.750000	0.750000	0.750000	0.750000	0.750000	0.750000
0.1	0.750918	0.750562	0.750434	0.750333	0.750144	0.750063
0.2	0.759857	0.755101	0.752681	0.751432	0.750850	0.750705
0.3	0.781564	0.769903	0.752073	0.757250	0.754745	0.754312
0.4	0.801291	0.788894	0.778031	0.769840	0.765064	0.764262
0.5	0.802632	0.797145	0.790577	0.783727	0.778996	0.778178
0.6	0.777870	0.786673	0.789724	0.789326	0.787909	0.787600
0.7	0.751081	0.765359	0.775806	0.782252	0.785191	0.785579
0.8	0.742099	0.750541	0.760088	0.768244	0.773070	0.773787
0.9	0.756646	0.753497	0.755007	0.758525	0.761333	0.761754
1.0	0.779124	0.769276	0.763094	0.760040	0.758885	0.758676
1.1	0.786955	0.781348	0.774839	0.769323	0.765921	0.765331
1.2	0.771312	0.776823	0.777538	0.775858	0.773955	0.773578
1.3	0.745202	0.758311	0.767011	0.771828	0.773728	0.773952
1.4	0.731475	0.741505	0.751455	0.759334	0.763772	0.764422
1.5	0.741784	0.740727	0.743897	0.748468	0.751772	0.752268
1.6	0.765842	0.755742	0.750199	0.748022	0.747493	0.747338
1.7	0.780854	0.771944	0.763649	0.757386	0.753788	0.753175
1.8	0.772458	0.773768	0.771107	0.767090	0.763952	0.763384
1.9	0.747904	0.753977	0.765067	0.767487	0.767869	0.767849
2.0	0.729379	0.740703	0.750540	0.757605	0.761289	0.761811
2.1	0.733591	0.735359	0.740430	0.746022	0.749720	0.750272
2.2	0.756399	0.747534	0.743653	0.742963	0.743345	0.743385
2.3	0.776611	0.765766	0.756933	0.750888	0.747648	0.747100
2.4	0.775459	0.773069	0.767799	0.762218	0.758359	0.757684
2.5	0.753848	0.762543	0.766044	0.766290	0.765368	0.765142
2.6	0.731520	0.743711	0.753100	0.759159	0.762015	0.762398
2.7	0.728897	0.733760	0.740720	0.747212	0.751201	0.751792
2.8	0.743304	0.741731	0.740160	0.741293	0.742719	0.742923
2.9	0.771824	0.760279	0.751832	0.746727	0.744243	0.743821
3.0	0.777773	0.772131	0.764920	0.758423	0.754268	0.753554
3.1	0.760632	0.766476	0.767319	0.765546	0.763491	0.763088
3.2	0.736118	0.748392	0.756764	0.761482	0.763362	0.763585
3.3	0.726725	0.734464	0.742911	0.749911	0.753940	0.754529
3.4	0.741081	0.737463	0.738456	0.741427	0.743839	0.744196
3.5	0.765942	0.754602	0.747460	0.743791	0.742305	0.742045
3.6	0.778442	0.770101	0.761618	0.754799	0.750714	0.750020
3.7	0.767072	0.769689	0.767889	0.764303	0.761308	0.760760
3.8	0.742271	0.753730	0.760489	0.763545	0.764323	0.764367
3.9	0.726831	0.736882	0.746205	0.753202	0.756968	0.757506
4.0	0.734937	0.734624	0.738157	0.742770	0.745989	0.746468
4.1	0.759129	0.740023	0.743732	0.741827	0.741467	0.741338
4.2	0.777159	0.766832	0.757797	0.751220	0.747549	0.746926

4.3	0.77244	0.771572	0.757412	0.752525	0.750555	0.751555
4.4	0.740315	0.759087	0.763731	0.764935	0.764522	0.764331
4.5	0.729033	0.740643	0.750133	0.756591	0.759794	0.760236
4.6	0.730242	0.733295	0.739116	0.745023	0.748792	0.749352
4.7	0.751328	0.743794	0.740805	0.740832	0.741626	0.741730
4.8	0.773943	0.762486	0.753644	0.747867	0.744881	0.744375
4.9	0.776253	0.772183	0.765827	0.759659	0.755561	0.754852
5.0	0.756632	0.763958	0.766151	0.765363	0.763846	0.763526

ME	INPUT SIGNAL	OUTPUT SIGNAL
0.0	0.750000	0.750000
0.1	0.960368	0.750063
0.2	0.977324	0.750705
0.3	0.785280	0.754312
0.4	0.560799	0.764262
0.5	0.510269	0.778178
0.6	0.680146	0.787600
0.7	0.914247	0.785579
0.8	0.997340	0.773787
0.9	0.853030	0.761754
1.0	0.613995	0.758676
1.1	0.500002	0.765331
1.2	0.615857	0.773578
1.3	0.855042	0.773952
1.4	0.997652	0.764422
1.5	0.912572	0.752268
1.6	0.678024	0.747388
1.7	0.509651	0.753175
1.8	0.562253	0.763384
1.9	0.787469	0.767849
2.0	0.978236	0.761611
2.1	0.959164	0.750272
2.2	0.747787	0.743385
2.3	0.538445	0.747100
2.4	0.523605	0.757684
2.5	0.716912	0.765142
2.6	0.940640	0.762398
2.7	0.939094	0.751792
2.8	0.817726	0.742923
2.9	0.584092	0.743821
3.0	0.502992	0.753554
3.1	0.648991	0.763088
3.2	0.887857	0.763585
3.3	0.999978	0.754529
3.4	0.882271	0.744196
3.5	0.642954	0.742045
3.6	0.502055	0.750020
3.7	0.539115	0.760760
3.8	0.824092	0.764367
3.9	0.990949	0.757506
4.0	0.936278	0.746468
4.1	0.710344	0.741388
4.2	0.520870	0.746926
4.3	0.542056	0.757980
4.4	0.754425	0.764381
4.5	0.962726	0.760236
4.6	0.975447	0.749352
4.7	0.780893	0.741730
4.8	0.557936	0.744375
4.9	0.511562	0.754852
5.0	0.684406	0.763526

APPENDIX G

LISTINGS OF VARIOUS SUBROUTINES

The subroutines listed in this appendix are:

1. TRANS
2. JACOBI
3. CHECK
4. SEMIAN
5. LINECT
6. CALCU
7. INTERP
8. ALI
9. ATSG
10. CS006A

The subroutines ALI and ATSG have been taken from "SCIENTIFIC SUBROUTINE PACKAGE (360A - CM - 03X). VERSION II PROGRAMMER'S MANUAL".

ALI is used for interpolation and ATSG is the subroutine for ordering the table from where the interpolation is to be done. The reference to these subroutines can be made to the above manual on page 253 for ATSG and page 245 for ALI.

The subroutine CS006A is new addition to the library and this was written by MRS. M. EASTON, Department of Computing Science, University of Alberta, Edmonton. This subroutine is used to find out the eigenvalues and eigenvectors of a real unsymmetric matrix.


```

SUBROUTINE TRANS(N,DX,D,MATRIX)
C   THIS SUBROUTINE CONVERTS THE ORIGINAL COEFFICIENT
C   MATRIX TO THE REAL SYMMETRIC FORM USING
C   SIMILARITY TRANSFORMATION
C   INPUT DATA
C   DX= THE GRID SPACING
C   N= THE NUMBER OF GRID POINTS
C   D=THE DIAGONAL MATRIX ,WITH DIAGONAL ENTERIES
C   HAVING ALTERNATE SIGNS I.E.  $D(I,I)=(-1)**(I)(D(I,I))$ 
C   USED FOR SIMILARITY TRANSFORMATION
C   MATRIX= THE ORIGINAL COEFFICIENT MATRIX (DIAGONALLY
C   DOMINANT & UNSYMMETRIC), DESTROYED DURING
C   COMPUTATION AND THE RESULTANT MATRIX IS SYMMETRIC
C   AND DIAGONALLY DOMANANT.
REAL*8 DX,ALPHA,BETA
DOUBLE PRECISION D(40,40),MATRIX(40,40)
ALPHA=0.2
BETA=DX/2.0
D(1,1)=1.0

C
C   CALCULATE THE DIAGONAL ELEMENTS OF MATRIX D.
C
NN=N-1
DO 100 I=1,NN
  II=I+1
  D(II,II)=D(I,I)*DSQRT((ALPHA+BETA)/(ALPHA-BETA))
100 CONTINUE
DO 102 I=1,20,2
  D(I,I)=-D(I,I)
102 CONTINUE

C
C   CALCULATE THE COEFFICIENT MATRIX CONVERTED INTO
C   THE SYMMETRIC ONE
C
DO 101 I=1,N
  DO 101 J=1,N
    MATRIX(I,J)=(MATRIX(I,J)*D(J,J))/(D(I,I))
101 CONTINUE
RETURN
END

```



```

SUBROUTINE JACOBI(N,MATRIX,VECTOR,TOLERC,NORM)
C JACOBI EVALUATES THE EIGEN VALUES AND EIGEN VECTORS
C OF A SYMMETRIC MATRIX
C INPUT DATA
C N=ORDER OF THE MATRIX
C MATRIX=THE MATRIX ITSELF
C VECTOR=MATRIX OF EIGEN VECTORS
C TOLERC=TOLERANCE LIMIT, INTERNALLY SET IF
C NOT SPECIFIED
C NORM=SPECIFIES THE TYPE OF NORMALISATION OF THE
C EIGENVECTORS. IF THIS IS 2, ORTHONORMAL EIGEN
C VECTORS ARE OBTAINED
DOUBLE PRECISION SINE,COSINE,TS1,TS2,LAMBDA,MU,
1 OMEGA,TOLERC, MATRIX(40,40), VECTOR(40,40),TS3
INTEGER I,J,P,Q,N,NM1,PP1,DONE,NORM
IF(TOLERC.EQ.0.000000000000) TOLERC=0.0000000000001
NM1=N-1
DO 1 I=1,N
DO 1 J=1,N
VECTOR(I,J)=0.0000000000000000
IF(I.EQ.J) VECTOR(I,I)=1.0000000000000000
1 CONTINUE
2 DONE=0
DO 5 P=1,NM1
PP1=P+1
DO 5 Q=PP1,N
IF(DABS(MATRIX(P,Q)).LE.TOLERC) GO TO 5
DONE=1
LAMBDA=-MATRIX(P,Q)
MU=.5000000000000000*(MATRIX(P,P)-MATRIX(Q,Q))
OMEGA=LAMBDA/DSQRT(LAMBDA*LAMBDA+MU*MU)
IF(MU.LT.0.0000000000000000) OMEGA=-OMEGA
SINE=OMEGA/DSQRT(2.0000000000000000+2.0000000000000000*
1 DSQRT(1.0000000000000000-OMEGA*OMEGA))
COSINE=DSQRT(1.0000000000000000-SINE*SINE)
DO 4 I=1,N
IF(I.EQ.P.OR.I.EQ.Q) GO TO 3
TS1=COSINE*MATRIX(P,I)-SINE*MATRIX(Q,I)
TS2=SINE*MATRIX(P,I)+COSINE*MATRIX(Q,I)
MATRIX(P,I)=TS1
MATRIX(Q,I)=TS2
MATRIX(I,P)=TS1
MATRIX(I,Q)=TS2
3 TS1=VECTOR(I,P)*COSINE-VECTOR(I,Q)*SINE
TS2=VECTOR(I,P)*SINE+VECTOR(I,Q)*COSINE
VECTOR(I,P)=TS1
4 VECTOR(I,Q)=TS2
TS1=MATRIX(P,P)*COSINE*COSINE-2.0000000000000000*
1 MATRIX(P,Q)*COSINE*SINE+MATRIX(Q,Q)*SINE*SINE
TS2=MATRIX(P,P)*SINE*SINE+2.0000000000000000*MATRIX(P,

```



```

1 Q)*COSINE*SINE+MATRIX(Q,Q)*COSINE*COSINE
  TS3=(MATRIX(P,P)-MATRIX(Q,Q))*SINE*COSINE+MATRIX(P,Q
1)* (COSINE*COSINE-SINE*SINE)
  MATRIX(P,P)=TS1
  MATRIX(Q,Q)=TS2
  MATRIX(P,Q)=TS3
  MATRIX(Q,P)=TS3
5 CONTINUE
  IF(DONE.NE.0) GO TO 2
  IF(NORM.NE.1) GO TO 8
  DO 7 J=1,N
    TS1=VECTOR(I,J)
    DO 6 I=2,N
      IF(DABS(TS1).LT.DABS(VECTOR(I,J))) TS1=VECTOR(I,J)
6 CONTINUE
    DO 7 I=1,N
      VECTOR(I,J)=VECTOR(I,J)/TS1
7 CONTINUE
    RETURN
8 DO 11 J=1,N
  TS1=0.0000000000000000
  DO 9 I=1,N
    TS1=TS1+VECTOR(I,J)*VECTOR(I,J)
9 CONTINUE
  TS1=1.0000000000000000/DSQRT(TS1)
  DO 10 I=1,N
    VECTOR(I,J)=VECTOR(I,J)*TS1
10 CONTINUE
11 CONTINUE
  RETURN
  END

```



```
      SUBROUTINE CHECK(VECTOR,MATRIX,N,W)
C      THIS SUBROUTINE MAKES A SIMILARITY TRANSFORMATION.
      DOUBLE PRECISION VECTOR(40,40),MATRIX(40,40),
1W(40,40)
      DO 400 J=1,N
      DO 400 I=1,N
      W(I,J)=0.0
      DO 400 K=1,N
      W(I,J)=W(I,J)+VECTOR(I,K)*MATRIX(K,K)*VECTOR(J,K)
400  CONTINUE
      RETURN
      END
```



```

SUBROUTINE SEMIAN(N,VAR,VECTOR,C1,C1,MATRIX,TIME
1,NT,CEVR,VICTOR)

```

```

C
C   THIS SUBROUTINE USES THE SEMI-ANALYTICAL SOLUTION
C   TO EVALUATE THE CONCENTRATION PROFILES AT
C   VARIOUS ELAPSED TIMES.
C
  REAL*8 CONST
  DOUBLE PRECISION VAR(40),VECTOR(40,40),C1(40),
1C1(40),MATRIX(40,40),TIME(40),CEVR(40,40),
2VICTOR(40,40)
  DO 8 J=1,N
    VAR(J)=0.0
    DO 8 K=1,N
      VAR(J)=VAR(J)+VICTOR(J,K)*C1(K)
8 CONTINUE
  DO 9 J=1,N
    C1(J)=VAR(J)
    DO 10 J=1,N
      VAR(J)=0.0
      DO 10 K=1,N
        VAR(J)=VAR(J)+VICTOR(J,K)*C1(K)
10 CONTINUE
  DO 11 J=1,N
    C1(J)=VAR(J)
    DO 13 J=1,NT
      DO 15 K=1,N
        CONST=-MATRIX(K,K)*TIME(J)
15 VAR(K)=((MATRIX(K,K)*C1(K)-C1(K))*DEXP(CONST)+C1(K))
        1/MATRIX(K,K)
      DO 17 L1=1,N
        CEVR(J,L1)=0.0
      DO 16 L2=1,N
16 CEVR(J,L1)=CEVR(J,L1)+VECTOR(L1,L2)*VAR(L2)
17 CONTINUE
18 CONTINUE
  RETURN
  END

```


SUBROUTINE LINECT(LINES,N,REFER)

C

C

C

C

C

THIS SUBROUTINE KEEPS A TRACK OF THE NUMBER OF
LINES PRINTED AND SKIPS TO A NEW PAGE LEAVING
SUFFICIENT MARGIN

INTEGER LINES ,N,REFER

LINES=LINES+N

IF(LINES.GT.61) GO TO 5

RETURN

5 WRITE(6,1)

LINES=9

IF(REFER.EQ.1) GO TO 6

RETURN

6 WRITE(6,2)

LINES=10

1 FORMAT(1H2,10X,8H ..CONTD)

2 FORMAT(1H,10X)

RETURN

END


```
SUBROUTINE CALCU(NN,N,NT,CEVR,CAPX,X,TIME,CGRID,XX)
```

```
C  
C THIS SUBROUTINE CALCULATES THE INTERPOLATED  
C VALUES FOR VARIOUS TIMES  
C
```

```
REAL CEVR(15,10),CAPX,X(5),TIME(15),CGRID(15,5),  
1XX(15),CPRIME(150)
```

```
DO 182 J=1,NT
```

```
DO 181 KA=1,N
```

```
DO 183 K=1,NN
```

```
CPRIME(K)=CEVR(J,K)
```

```
183 CONTINUE
```

```
CALL INTERP(10,X,XX,CPRIME,KA,CC,N,NT)
```

```
CGRID(J,KA)=CC
```

```
181 CONTINUE
```

```
182 CONTINUE
```

```
RETURN
```

```
END
```


SUBROUTINE INTERP(NP,X,XX,Y,KA,CC,N,NT)

INTERP USES THIRD ORDER LAGRANGIAN INTERPOLATION
FORMULA. THE INTERPOLATED VALUE IS CC.

REAL X(5),XX(15),Y(150),CC

DO 202 KB=1,NP

IF(X(KA).GT.XX(KB)) GO TO 202

GO TO 203

202 CONTINUE

203 LA=KB-2

IF(LA.EQ.0) LA=1

LB=KB+1

IF(KB.EQ.NP) LB=NP

CC=0.0

DO 207 KC=LA,LB

RP=1.0

DO 206 KD=LA,LB

IF(KD.EQ.KC) GO TO 205

RS=(X(KA)-XX(KD))/(XX(KC)-XX(KD))

RP=RP*RS

GO TO 206

205 RS=1.0

206 CONTINUE

RP=RP*Y(KC)

207 CC=CC+RP

RETURN

END

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